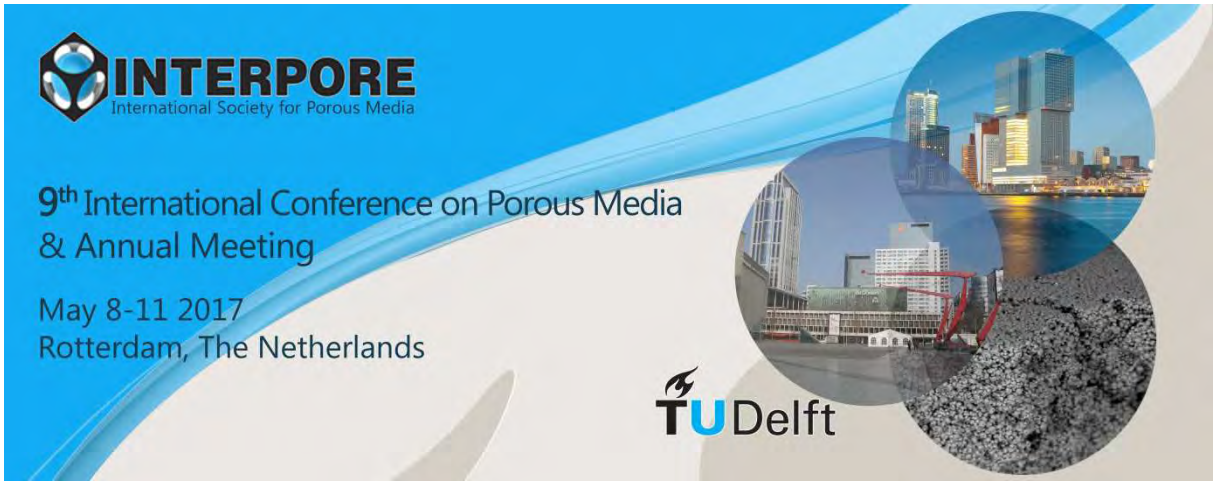

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Book of Abstracts

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A domain decomposition approach to volume averaging with application to non-Fickian transport

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Homogenized models, where microscopic details are filtered out to reduce numerical and physical complexity, are often used to describe transport phenomena in multiscale multiphase materials and porous media. An important aspect of adopting such a macroscopic point of view is that there is generally not a one-to-one correspondence between the microscale problem and the macroscale model: for a unique microscale problem, there exists a variety of homogenized models. For instance, either a one- or two-temperature model may be used to describe heat transfer by advection and diffusion in a medium containing two different phases. Depending on the geometry of the domain, the boundary conditions, the time regime of interest or the value of the dimensionless parameters in the partial differential equations (PDEs), either one mathematical model or the other will be more adapted. This situation stems from the fact that macroscale models rely on different approximations and, therefore, have different domains of validity. One-temperature models, for example, require some relaxation (e.g. local equilibrium, time-asymptotic) of the temperature fields between the two phases, whereas two-temperature models capture a characteristic time associated with heat exchange between the two phases (see [1,2]). In the volume averaging framework for upscaling, multi-equation models can be obtained by a domain decomposition approach where the spatial domain is decomposed into several subdomains and averaging operators are applied to each domain separately. Exchange terms at the macroscale characterize exchanges that occur at the microscale through the transmission boundary conditions connecting the PDEs of different subdomains. This approach is generally used to describe systems with clearly distinct materials, such as a fluid and a solid phase, where transport properties vary significantly. Interestingly, even a unique physical phase can feature sub-regions with different properties, such as fluid flow in a porous medium with preferential channels [3] and dead-end pores. For solute transport, these differences in the properties of the two regions may generate non-Fickian transport, such as heavy-tailed breakthrough curves, similarly to a configuration with multiple phases. In this work, we focus on a generic pore-scale problem of transport by advection and diffusion. We show that the spatial domain can be decomposed in any number N of subdomains and use the method of volume averaging to obtain the corresponding N-equation model at the macroscale. This homogenized description quickly gains in complexity with the number N, as the model captures more characteristic times of the microscale transport problem and provides a more accurate description of the processes. We illustrate this issue using computational results comparing models with increasing N and direct numerical simulations at the microscale. We also discuss the problem of optimal domain decomposition, give examples of domain decomposition and provide perspectives on the application of this approach.

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A theoretical study of Streamline Reservoir Simulation for incremental oil recovery by water flooding process using FrontSim

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Abstract: Average worldwide oil recovery per reservoir is estimated at 38%.The interplay of reservoir drive mechanisms and complex geology accounts for most un-recovered oil & gas. Streamline technology is a rapidly evolving technology aimed to meet the demands of high resolution simulation designed for large, heterogeneous and geologically complex reservoir models. FrontSim is a 3-phase Black Oil streamline reservoir simulator that shares a similar user interface with other simulators in the ECLIPSE suite. FrontSim models the flow of fluids along streamlines. In this paper, about Waterflood process, FrontSim provides some interesting and unique features that have been proved to be very beneficial in reservoir management by means of Pattern Flood Management (PFM) in the Data file. According to what has been shown at the end of this paper, in the example reservoir that water flood has been applied in it, the location with lack of drainage area intersection of all the injection and production wells, the un-swept location can be a good candidate for infill drilling another production well for incremental oil recovery in this reservoir.

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Adsorption and hydrodynamics in nanochannels: towards tunable membranes

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We study the flow of a near-critical mixture through a nanopore in contact with two material reservoirs. At equilibrium, the pore walls interact favourably with one of the mixture components and we recover the well-known picture of critical adsorption [1]. However, when the fluid velocity through the pore increases, the interplay between advection and diffusion, or Péclet number, leads to two intriguing steady-states. Initially, we find that the pore acts a weakly selective membrane, separating the critical mixture components at an extremely low pressure. Upon further increase of the pressure, advection becomes dominant leading to a depletion of the pore composition, described by a simple shift of the adsorption. We present numerical and analytical results explaining these phenomena which could be reversibly controlled by the application of an external pressure as well as temperature [2].

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Advection-diffusion in porous media at low scale separation via higher-order homogenization

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Asymptotic multiple scale homogenization allows to determine the effective behaviour of a porous medium by starting from the pore-scale description. The thus obtained continuum descriptions are valid when the given phenomenon is considered in a medium with a large number of heterogeneities. This hypothesis of separation of scales means that the macroscopic size L, is very large in comparison with the size l of the heterogeneities. It is therefore interesting to investigate how the described theories are modified when the hypothesis of scale separation is not perfectly respected. This happens when the porous medium is macroscopically heterogeneous or when large gradients are applied to macroscopically homogeneous media. The asymptotic multiple scale homogenization method is particularly well adapted to this type of analysis. The effect of low scale separation can be obtained by exploiting higher order equations in the asymptotic homogenization procedure and then by analyzing their role in the macroscopic description. Higher-order homogenization thus allows both the determination of the conditions under which the influence of the microstructure is negligible and also how the microstructure may modify the response of the medium. While higher-order homogenizaton has been been widely applied in the field of mechanics of composite materials (e.g. (Gambin and Kröner, 1989), (Boutin, 1996)), porous media at low scale separation have received very little attention. However, an important work is presented in (Goyeau et al., 1997), where the method of volume averaging is used to obtain the correctors of Darcy's law. The same problem is tackled via higher-order homogenization and up the third order in (Auriault et al., 2005). The aim of the present study is to investigate higher-order terms of the advective-diffusive model to describe advection-diffusion in a macroscopically homogeneous porous medium at low scale separation. The advective-diffusive model is obtained by first-order homogenization when considering the convection-diffusion equations with a macroscopic Peclet number (i.e. the Peclet number measured by means of the macroscopic length L) in the order of 1 on the pore scale (Auriault and Adler, 1995). The second and third order models are derived. The main result of the study is that the low separation of scales induces dispersion effects. In particular, for a macroscopically homogeneous medium, the second-order model is similar to the most currently used phenomenological model of dispersion: it is characacterized by a dispersion tensor which can be decomposed into a purely diffusive component and a mechanical dispersion part, whilst this property is not verifed in the homogenized dispersion model (obtained at higher Peclet numbers). The third-order description contains second and third concentration gradient terms, with a fourth order tensor of diffusion and with a third-order and a second-order tensors of dispersion.

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Description of Quasi Static and Quasi Stationary Processes of Capillary Transport of Liquid in Unsaturated Porous Materials

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Description of the quasi static and quasi stationary processes of capillary transport of liquid and gas is presented in the paper. It is the second part of the manuscript published in Meccanica, [2], in which the new macroscopic description of the capillary transport of liquid and gas in porous materials is proposed. In the manuscript model assumptions for the proposed description and the kinematics of the system components were discussed in detail and balance equations for mass, momentum and internal energy of the whole system were formulated. Theoretical considerations were performed within the framework of multi-phase continuum mechanics. Gas and liquid filling a non-deformable porous material is assumed to form a macroscopic continuum consisting of three components: gas, mobile liquid and capillary liquid, while the matrix is non-deformable with isotropic and homogeneous pore space structure. The capillary liquid is immoveable, form a thin layer on the pore surface and exchange mass, linear momentum and energy with the mobile liquid in the vicinity of the menisci surfaces, the movement of which is described by an additional velocity field. In the present paper a new definition of the quasi static process and a new class of quasi stationary processes is proposed in which boundary conditions change quasi statically. This allows one to use the results of the first part of the considerations and to derive equations describing quasi-static and quasi-stationary macroscopic processes of liquid and gas transport in porous materials. This concerns e.g. description of mercury intrusion into porous materials, which plays important role in the mercury porosimetry as a theoretical basis for data interpretations, [1]. In turn, the obtained equations for quasi stationary processes can be used to describe the flow of viscous liquid and gas through porous materials. It was shown that in both cases equations are strongly nonlinear and their solution needs the advanced analytical and numerical methods to be applied. Even relatively simple problem of non-wetting fluid flow through the layer of porous material is described by the system of three nonlinear strongly coupled equations for fields of velocity, saturation and pressure in the fluid.

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Dynamic adsorption-diffusion model for modeling gas production in shale

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Reliable mathematical model for analysis of shale gas production requires to consider gas storage form in shale rocks: free gas in micro- and nano- scale pore, adsorbed gas on the surface of organic matter and clay mineral and dissolved gas molecules in kerogen. A so-called dynamic adsorption-diffusion (DAD) model is presented, in this paper, to analyze the production process in shale rocks. This model considers that the adsorption/desorption process of adsorbed gas is a time-dependent instead of instantaneously reaching equilibrium, meanwhile the diffusion process of dissolved gas in kerogen is also taken into account. The general analytical solution for DAD model is derived. The dynamic adsorption/desorption parameters (adsorption/desorption rate coefficient) are estimated through matching the analytical solution of DAD model with the experimental results of shale gas production process under laboratory condition. The parameter estimation method is realized by a global optimization method, called multilevel single-linkage (MLSL) method. The critical points, which distinguish the domination stage of free gas, desorbed gas and dissolved gas, are determined in a mathematical way through using DAD model and dissolved gas model. The experiment for DAD model is conducted under constant pressure boundary condition. The recorded data is the accumulated production gas volume under standard condition. The DAD model can match with the experimental results well. The gas production process can be divided into three stages: free gas production domination stage, adsorbed gas domination stage and dissolved gas domination stage. The time range for the first production stage is small, but its production rate is large. And production stage for adsorbed gas and dissolved gas lasts long time, but the production rate for these two stages are much smaller than the first stage. The length of time for these three stages is: free gas stage<adsorbed gas stage<dissolved gas stage. The time for the stage of adsorbed gas production will be extended when the dynamic parameters decrease. The diffusion coefficient for gas diffusion in kerogen is very small. The DAD model presented in this paper can not only be applied in characterizing gas production under laboratory conditions, but also can be applied in reservoir conditions. With the dynamic coefficients obtained from the laboratory test, the dynamic gas transport curves can be calibrated to actual well performance in shale gas reservoirs, leading to improved understanding and forecasting of the shale reservoir.

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Ensemble Distribution for Immiscible Two-Phase Flow in Two-Dimensional Networks

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An ensemble distribution has been constructed [1] to describe steady immiscible two-phase flow of two incompressible fluids in a network of pores. The system is ergodic. The distribution relates the time that a bubble of the non-wetting fluid spends in a link to the local volume flow. The properties of the ensemble distribution are tested by two-phase flow simulations at the pore-scale for capillary numbers ranging from 0.1 to 0.001. It is shown that the distribution follows the postulated dependence on the local flow for Ca = 0.01 and 0.001. The distribution is used to compute the global flow performance of the network. In particular, we find the expression for the overall mobility of the system using the ensemble distribution. The entropy production at the scale of the network is shown to give the expected product of the average flow and its driving force, obtained from a black-box description. The distribution can be used to obtain macroscopic variables from local network information, for a practical range of capillary numbers.

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Fluid-Solid interactions for atoms and particles

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The interactions of fluids and solids has many aspects and involves a multitude of mechanisms and phenomena at multiple scales. The focus of this presentation is on three of those: 1) the transition from a solid to a fluid (e.g. relevant for the release of avalanches and landslides) as well as the transition from a fluid to a solid-like behavior (related to jamming and shear-thickening in various materials like suspensions or soft and granular matter. 2) the interaction of a fluid with the solid boundaries, which leads to short-ranged ordering, layering or crystallization, e.g. a wall-induced microstructure that renders the fluid behaving much differently from a bulk-fluid due to the existence of this fabric/structure on the atomistic or particle scale. 3) the interaction between a fluid flowing through a complex structure and the microstructure of the porous material, where in understanding the relations between porosity, permeability and microstructural feaers is the goal.

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Impact of Invasion Percolation on Upscaling in Capillary-Controlled Darcy-scale Flow

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The steady-state method is one of the main approaches to upscale multiphase flow properties in Darcy-scale simulation. The computation of effective quantities, namely relative permeabilities and capillary pressures, may become, however, computationally very demanding when accounting for the combined effects of viscous, buoyancy and capillary forces. Nevertheless, under certain flow conditions, computations are greatly simplified and fluid saturations, which are essential in calculating average properties, can be estimated from local multiphase flow parameters. In capillary-dominated displacements, for instance, fluid saturations are determined from local capillary pressure curves. In a heterogeneous capillary-controlled environment, a phase may fail to form a connected path across a given domain at capillary equilibrium. Moreover, even if a continuous saturation path exists, some regions of the domain may produce disconnected clusters that do not contribute to the overall connectivity of the system. In such cases, conventional upscaling process might not be accurate since identification and removal of these isolated clusters are extremely important to the global connectivity of the system and the stability of numerical solvers. In this study, we address the impact of percolation during capillary-controlled displacements in heterogeneous porous media. We present a comprehensive investigation using random absolute permeability fields, for water-wet, oil-wet and mixed-wet systems, where J-function scaling is used to relate capillary pressure, porosity and absolute permeabilities in each grid-cell. Important information is revealed about the average connectivity of the phases and the trapping of saturations due to capillary forces.

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Impact of wettability at the pore scale flow regime

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Flow behavior and displacement efficiency during immiscible displacement in porous rock is significantly influenced by the wettability of the fluid-rock system. This has a large impact on many multiphase flow problems, for instance during oil recovery. Various studies on core-floods showed the dependence of oil production and the relative permeability on the wettability of a rock [1,2]. However, core flooding experiments do usually not give access to the details of the underlying processes at pore scale. Micro computed tomography provides the facility to investigate the oil distribution inside the porous rock in great detail. Iglauer et al. [3] visualized the different shapes of oil clusters in water wet and mixed wet systems. Andrew et al. [4] introduced a method to measure contact angle in-situ in porous media and Singh et al. [5] showed the change in fluid distribution while aging a sample from water wet towards oil wet. In this study we focus on the influence of wettability on the flow dynamics by directly observing the forced imbibition (flooding) in mixed-wet systems in sandstone and carbonate rock in real time and in 3D in by using synchrotron beamline-based fast X-ray computed

tomography. The micro-CT flow experiments were conducted at the TomCat beamline at the Swiss Light Source of the Paul-Scherrer-Institute. The flooding experiment was imaged in-situ in real-time at 7s scanning time. The 20mm long and 4mm wide rock samples were prepared in advance by saturating them first with brine containing 200g/l KI (which serves as doping agent as well) and then with crude. In order to establish mixed-wettability, the rock samples were “aged” by applying 30 bar pressure and 70C temperature for one week. The 3D images were analyzed with AVIZO and Geodict to determine event types as snap-off and coalescence to assess their contribution to the overall flow. The results show a ganglion dynamic flow behavior for mixed-wet systems. The oil filling events are more frequent, larger and slower compared to oil-filling events in water-wet imbibition [6] and show a strong dependency on the wetting stage of the surrounded surface. As such oil filling events are known to affect the oil-configuration in the rock and the connectivity of the oil phase [7] these behavior may impact the overall relative permeability and has to be considered in pore-scale flow simulations.

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Intermediate-wettability effects on two-phase flow in porous media

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Multiphase flow in porous media is important in a number of environmental and industrial applications such as soil remediation, CO2 sequestration and enhanced oil recovery. Wetting characteristics of porous media controls flow of immiscible fluids in porous media and phase distribution in the pore space. In contrast to the strong and weak wetting conditions, the pore scale physics of immiscible displacement at intermediate wetting conditions is less understood. This study reports the results of a series of two-dimensional high-resolution direct numerical simulations with the aim of understanding the dynamics of pore-scale fluid displacement events at intermediate-wet conditions. Our results show that for intermediate-wet porous media the complex interplay of pore geometry and surface forces induces co-existence of concave and convex interfaces revealing previously unidentified features including i) pinning of convex interfaces, ii) reverse displacement, and iii) interface instability. Moreover, we explored the dynamics of blob as affected by the interface coalescence under intermediate-wet conditions. These pore scale events significantly influence macroscale flow behaviour causing the counter-intuitive decline in displaced fluid recovery as the strength of capillary forces decreases from weak imbibition to intermediate-wet conditions.

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Numerical Simulation for Convection Heat Transfer in Sintered Porous Media Channels with an Improved Local Thermal Non-Equilibrium Model

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Heat transfer in porous media has received much attention for many years due to its importance in engineering. There are two primary ways to model the heat transfer process in porous media: the local thermal equilibrium (LTE) model and the local thermal non-equilibrium (LTNE) model. The LTE model neglects the interphase temperature difference, while the LTNE model is more accurate since it accounts for the interphase temperature difference. Recently, several improvements have been made for the LTNE model, e.g., thermal boundary condition models, effective thermal conductivities, internal heat transfer coefficients and etc. The present work conducts numerical simulations for convection heat transfer in channels filled with sintered porous media (Figure 1), using a local thermal non-equilibrium model with improvements on the thermal boundary condition model [1] and the effective thermal conductivity model [2]. Using the LTNE model with the improved thermal boundary condition model and effective thermal conductivity model, the present work calculates the experimental cases of Jiang et al. [3] and compares the results with the previous model, the partially improved model and the experimental data. The comparisons show good agreements between the present model and the experimental data. Since the improved models in the present model are general and reasonable, the improvements can be extended to other investigations with the local thermal non-equilibrium model.

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On the Use of Distribution Functions to Determine Signatures of Flow, Transport and Reactive Processes

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Understanding of flow, transport and reaction processes in the subsurface has been transformed by the advances in both X-ray imaging and pore-scale modelling. A digital rock analysis methodology based on distribution functions is demonstrated as a novel tool in determining the signatures of flow, transport and reaction in subsurface rock. The key advantage is that pore space geometry is described by the statistics routinely consisting of - 10^9 voxels.

This concept is illustrated by using the simulation of flow, transport and reaction processes on micro-CT images of a beadpack, a sandstone, and a carbonate, representing porous media with an increasing degree of pore-scale complexity. Exemplar applications that characterise impact of heterogeneity include single phase fluid flow, solute transport, fluid/fluid reactive transport, and fluid/solid reactive transport. This is illustrated in Fig.1 in which distributions of solute displacements obtained by model for beadpack, sandstone and carbonate are compared with independently acquired NMR measurements, and in Fig.2 where voxel distributions in which reaction has occurred are compared for beadpack and two sandstones. By establishing analysis that uses distributions, spatial information on transport and reactive processes is retained, which offers a more detailed description in comparison to approaches that rely on average quantities. This methodology enables us to underpin modelling results with micro-CT imaging experiments and/or NMR experiments at multiple scales.

The wealth of pore-scale information enables us to introduce new quantitative characterisation of flow/transport/reaction -based heterogeneity of subsurface rock. Moreover, novel methodologies are now being developed for utilising this information at larger scales by a simultaneous application of X-ray tomography and NMR measurements, and multi-scale reactive transport modelling.

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Path Integral Method for Flow through Random Porous Media

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The permeability of a reservoir rock describes the resistance to fluid flow: it relates the local flow rate to the local pressure gradient. The aim of any model describing flow through a porous medium is to generate simulations of the pressure in accordance with their probabilities of occurrence. For a realistic model it is necessary to have a three-dimensional representation of the geological heterogeneities K(x). We focus on the simplest case of single-phase, steady state flow. We use a stochastic model for the permeability K(x), characterised fully by its mean and covariance matrix. The form of K(x) is a simplifying assumption made for this work, but, in principle, the path integral is not restricted to a specific form when calculated numerically. The conventional way to calculate pressure statistics is through generation of explicit realisations of the geological model; the pressure field is found through the relation

$$\nabla.(K(x)\nabla p(x))=0,$$

obtained from Darcy's law and the continuity equation

$$\nabla. q(x)=0.$$

For a reliable estimate of the statistics of p(x) a considerable number of independent realisations of the inverse matrix of transmissibilities K(x)-1 is needed. An example of a number of pressure realisations, with the initial and final pressure fixed (‘Dirichlet boundary conditions’) is shown in Figure 1. In repeating the matrix inversion a large number of times one runs into heavy computational requirements.

We propose a method based on the path integral formalism as a computationally less demanding alternative. The path integral is widely used in branches of physics ranging from quantum mechanics to probability theory. It is an explicit formula for the probability amplitude associated with each ‘pressure trajectory’ from the initial to the final pressure. Casting the problem in path integral form has the advantage of access to existing techniques for path integrals, notably the renormalisation group and applications to perturbation theory. The method does not rely on the inversion of explicit permeability realisations. Rather, one works with the established stochastic model for the inverse permeability, characterised by its mean and covariance matrix. The path integral enables direct sampling from the pressure field p(x), subject to Darcy's law. This should decrease the computational demands associated with computing the pressure statistics. The pressure statistics resulting from the path integral approach are shown to be in very good agreement with those obtained through conventional methods for one-dimensional Darcy flow through a permeable medium (see Figure 2). An approximation based on a Gaussian model is provided. We emphasise that this approximation is designed as a rough fit; the data are a better representation of reality.

We believe the advantage of the path integral algorithm, the circumvention of the computationally demanding step of matrix inversion, to be greatest in three dimensions. The application of the path integral to three-dimensional Darcy flow is in progress.

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Study of the effect of resolution on transport properties of digital rocks using stochastic super-resolution technique

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Permeability is one of the fundamental properties of porous media and is required for large-scale Darcian fluid flow and mass transport models. Whilst permeability can be directly measured at a range of scales, there are increasing opportunities to evaluate permeability from pore-scale simulations. It is well known that single phase flow properties of digital rocks will depend on the resolution of the 3D pore image. Such studies are usually performed by coarsening X-ray microtomography scans. Recently we have proposed a novel approach to fuse multi-scale porous media images using stochastic reconstruction techniques based on directional correlation functions. Here we apply this sligthly modified approach to create 3D pore images of different spatial resoltuion, i.e. stochastic super-resolution method. Contrary to coarsening techniques, this approach preservs porosity values and allows to incorporate fine scale data coming from such imaging techniques as SEM or FIB-SEM. We compute absolute permeability of the same porous media species under diferent resolutions using lattice-Boltzmann and finite difference methods to model Stokes flow in order to elicidate the effects of image resolution on resulting permeability values and compare stochastic super-resoltuion technique against conventional coarsening image processing technique.

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Surfactant variations in porous media localize capillary instabilities during Haines jump.

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We use confocol microscopy to visualize thin film formation between a trapped phase with surfactant to a flowing phase in three dimensional porous medium. We find that viscous drag forces on the thin film can destabilize capillary forces in drainage and imbibtion, a process known as Haines jumps. Moreover, we show that viscous forces inhomogenously deplete surfactant leading to variations in interfacial tension and localizing capillary destabilization. Our results suggest that even in steady state flow with no variations of pressure the trapped phase can be moblized by the interplay of viscous to capillary forces.

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Two-Phase Flow in Porous Media - As Seen from Thermodynamics

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We argue that the steady-state two-phase flow in a porous isothermal medium can be viewed as an Euler homogeneous function of the first kind of the cross-sectional surface areas available to each component for any cross section [1]. From this mathematical property alone, it follows that we can write relations between the fractional flows of the two components and their degrees of pore saturation; this in complete analogy with thermodynamics. The machinery and tools of thermodynamics become available, and we can see that the generalized Darcy equations obey the overall structure provided by the new theory. The Corey model, however, does not give relations, which conform to the thermodynamic structure. We show that the relative permeability of one component can be derived from the permeability of the other component via a Gibbs-Duhem type equation, and that all work added to the system is consistent with the energy that is dissipated as heat. The theory can be generalized to non-isothermal conditions. These results simplify the number of measurements needed to give a complete description on the macroscopic level. Numerical results are presented to illustrate the use of the equations.

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Unraveling the Mechanism of Dynamic Emulsion Formation in Transparent Porous Medium Miocromodels

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The production of hydrocarbons from poor-quality petroleum resources such as unconventional tight reservoirs has become more prevalent in recent years. However, due to the heterogeneous nature of the reservoir rocks which are made of interconnected micro and nanosized pore –throats, the recovery factors are not still efficient even after primarily waterflooding. Chemical recovery methods provide opportunities to improve the oil displacement from rocks by breaking down the trapped oil in by-passed zones and through separating the residual oil from rock surfaces in form of small droplets suspended in water phase. In this work, a highly-transparent and mimetic-structure microfluidic platform is utilized to investigate the process of oil displacement using an aqueous phase flowing through synthetic microfluidic-based porous medium models made of constituting a network of 10 to 100 size microchannels. Micromodels are fabricated based on soft lithography techniques on silicon wafer and replicated with Polydimethylsiloxane (PDMinisymposium). Deionized water (DI) and complex fluids (i.e. suspensions of nanoparticles and surfactants) are used as aqueous phases for displacing oil with a wide range of viscosities ranging from 50 to 1000 cp. Consistent with the reported reservoir core scale experiments, the complex suspensions demonstrate an enhancement in the oil recovery in comparison with water flooding. It is revealed that the primary mechanism of mobilizing the residual oil during the complex fluid flooding is the formation of spontaneous oil in water emulsification inside microchannels (Graphics1-3). During the displacement process, the capillary and shear forces inside the microscale structures provide energy required for emulsification in the dynamic multiphase fluid system. To disclose the effect of shear forces on spontaneous emulsification, experiments are repeated with different flow rates. Results demonstrate that there is a minimum injection flow rate of 0.01ml/hr in a 10 micron sized channel to reach a critical shearing force required for mixing the phases and consequently emulsification. The developed microfluidic-based model is a powerful mimetic model of real porous media which can clarify the mechnaisms underlying the process of chemical-based flooding for oil recovery. Considering the time-consuming and expensive nature of coreflood experiments, the proposed microfluidic approach provides an attractive alternate for the rapid and low-cost enhanced oil recovery (EOR) screening studies.

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A conservative level set method for simulating two-phase flows in porous media

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Multiphase flows in porous media are of critical importance in a number of areas such as phase separation in engineering devices (e.g., coalescers) and carbon dioxide sequestration. Common challenges in these applications include – among others – the characterization of contact line motion within complex geometries and the physical discontinuities at the fluid-fluid interface and fluid-solid interface. In this talk, we present a computationally efficient methodology with emphasis on contact line modeling for simulating two-phase flows within complex geometries, which relies on an immersed boundary approach and on a conservative level set technique modified to account for contact line dynamics. This method is shown to be mass-conserving and accurate even at limited resolution. Then we use this newly developed computational approach to explore the physics of droplet interacting with rigid fibers, and two-phase flow displacement in porous media.

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A multiscale method for filter efficiency simulations

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We are interested in the dead-end depth filtration of contaminants out of air using non-woven filter media. In general, filtration is an intrinsically multiscale process. Hence, we use mathematical homogenization, which is an upscaling technique that models variations at macroscale while accounting for filtration processes at microscale. We use homogenization theory for fully coupled problems of: the fluid flow through the filter medium, the contaminant transport with convection, diffusion and adsorption and the evolution of the filter medium microstructure due to the contaminant adsorption [1]. To represent the non-woven filter medium we use different models for 2D microstructures: square grid, hexagonal grid and random distributions of fibres. First, we present the homogenization model and discuss how we account for the dust deposition for the different microstructure models. Then, we study the influence of the microstructure model on the permeability and effective diffusivity at microscale and on the filter efficiency at macroscale.

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A new algorithm for unstructured tetrahedral meshing of pore-scale digital images

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Image-based pore-scale modeling techniques have become widely used simulation tools. For flow modeling, the two dominant approaches are pore network modeling and the lattice Boltzmann method (LBM). In contrast, traditional methods for computational fluid dynamics or solid mechanics have not been widely used. Part of the reason for this is due to the benefits of network modeling and LBM for porous media problems. However, there is also a barrier to using methods that require mesh generation, especially in the case of complicated structures such as the pore space of natural heterogeneous materials. This barrier is unfortunate because techniques such as the finite element method can offer significant advantages for many problems including those that involve multiphysics and/or solid mechanics, flow of non-Newtonian fluids, and simulations that would benefit from unstructured grids and high levels of local refinement.

To help address this limitation, we have developed a new algorithm for tetrahedral mesh generation from digital images. It is designed particularly for pore-scale applications, but is flexible enough to be used for mixed-scale or continuum domains as well. The foundation for the algorithm is a fast point-insertion algorithm for Delaunay tessellation. By coupling the point-insertion with structural inputs (e.g., provided by the user, created form distance transforms, or taken from other inputs such as a pore network), we created an approach that controls the mesh structure, local refinement, and mesh quality in a robust, integrated manner. The algorithm has a number of differentiating factors, which include allowing the user to

• Incorporate both digital and geometric structures in the same domain • Provide highly flexible control of local mesh refinement. • Mesh tight internal structures (e.g., the pore space) at coarser resolutions than can be done with surface-based methods. • Provide a natural way to ignore small features and/or imaging artifacts if needed. • Either conform precisely to defined structures in the image or approximate surfaces to conform to global criteria such as porosity, surface area, smoothness, etc. • Specify mesh resolution independently of image resolution. • Specify spatial mesh resolution that spans many orders of magnitude, while still maintaining good control of element quality.

A series of examples are presented that illustrate the algorithm's performance. The chosen example are centered around particles in the pore space because of the wide range of applications to which this issue applies and because it effectively illustrates multi-resolution problems. These examples also illustrate important quantitative qualities such as automatic and user-imposed refinement, adapting to structural features in the image, and speed of the algorithm.

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Advanced nonlinear strategies for Operator-based Linearization Approach

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Convergence issues in the nonlinear solver of a reservoir simulator is common even when the Fully Implicit Method (FIM) is used to discretize the nonlinear conservation equations. Although FIM is unconditionally stable, it is not guaranteed to converge for large time steps due to the nonlinearity of the conservation equation, leading to unacceptably large computational time. A safeguard strategy such as the trust-region method proposed in Voskov and Tchelepi (2011) can help to improve the convergence performance of the general purpose simulation in cases where the highly nonlinear flow and transport are strongly coupled and have generally complex physics. We describe a new nonlinear solver strategy which is implemented within the operator-based linearization framework proposed by Khait & Voskov (2016). In this approach, the terms of the nonlinear conservation equation are presented as a product of two different operators: the first depends on the current physical state of the system (state-dependent) and the other contains the spatially altered properties (space-dependent). This operator splitting approach allows us to treat the nonlinear physics representation separately from the spatially altered properties in a fully coupled manner. During the course of simulation, the non-linear physics is approximated using a multi-linear interpolation based on the primary variables of the pressure and composition, in which its accuracy is controlled by the resolution of interpolation tables. Such separation and approximation of the original nonlinear physics in combination with an adaptive coarsening in parametrization space allows for the flux function to be segmented into trust regions. The key idea behind this strategy is that all special point (e.g. inflection points) in the generalized flux function can be adaptively computed and divided into trust-regions according to the interpolation points in the parametrized space. We use the Implicit Hybrid Upwinding (IHU) scheme presented by Hamon and Tchelepi (2016) to deal with the convection flux in the presence of buoyancy and capillarity. The proposed strategy can be seen as an extension of the trust-region Newton Solver proposed by Wang and Tchelepi, and resolves other features such as the different type of kinks present in a fractional flow curve (Li and Tchelepi 2015). The robustness and efficiency of our nonlinear solver is tested in several challenging compositional problems. In addition, the performance of our nonlinear strategy is compared against existing nonlinear solvers.

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Application of Smoothed Finite Element Methods in Solution of Coupled Hydro-Mechanical Problems

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The finite element method (FEM) has been used widely to solve many different problems. But, a major shortcoming of this method is its mesh dependency. By application of strain smoothing technic, smoothed finite element methods (SFEM) were created that overcome this shortcoming. These methods were created when stabilized conforming nodal integration, that was successfully applied in mesh-free methods to make them linearly consistent, was used in the FEM. In SFEMs, integration is performed on “smoothing domains”, rather than elements. After discretization of the problem domain into elements, these smoothing domains can be created based on cells, nodes, or edges, that in turn make Cell-based, Node-based or Edge-based smoothed finite element methods. These different methods, have different properties. SFEMs are insensitive to mesh distortion and are generally more computationally efficient than mesh-free and finite element methods for the same accuracy level. The node-based SFEM can give upper-bound solution, and while it is temporally unstable, the edge-based SFEM can give stable results that are ultra-accurate. Interesting features of SFEMs, have made them an efficient tool to solve many different problems [1]. In this paper, performance of SFEMs in solution of coupled hydro-mechanical (consolidation) problems based on the Biot’s theory is investigated. Different scenarios for application of smoothing technic in solution of consolidation problems are tested through some examples. Results are compared with FEM and analytical solutions to find the best and most efficient scenario. A number of facts has been considered in designing solution scenarios. First, it has been shown that strain smoothing technic will give erroneous results when using quadratic or higher order shape functions [2]. So, application of the Babuška-Brezzi condition is impossible using SFEMs. On the other hand, node-based SFEM can give results which are “softer” than exact solution, that can solve the oscillations due to volumetric locking problem of water. Also, edge-based SFEM can give results that are as accurate as FEM results using higher order shape functions. Another fact is that the FEM can be combined with SFEM and only one phase of the coupled domain, rather hydraulic or mechanical, be smoothed. Combination of all these facts, makes different scenarios. Through investigation of all results, shows that the best and most efficient scenario is to combine the FEM and SFEM. Using this method, the Babuška-Brezzi condition can be applied that prevents numerical instabilities. Also, it has been shown that the combined FEM-SFEM method gives more accurate results and is more computationally efficient in comparison to using only the FEM method.

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Coupling Deformation and Flow in Fractured Poroelastic Media: Modelling, Analysis and Simulation

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Coupled fluid–solid interaction processes in fractured porous media play an important role in engineering applications such as the design and construction of geothermal power plants, the risk assessment of waste deposits, and the production of crude oil and gas. Numerical simulation of these processes remains challenging due to the number of physical processes involved, the nonlinear coupling, the complex geometries, and the hetereogeneous nature of fractured porous rock.

In this work we focus on the nonlinear coupling between hydrology and mechanics. We introduce system of PDEs for the modeling the coupling of deformation and flow in a domain with a stationary fracture. The fluid flow in the fracture is modeled by a lower-dimensional equation, which interacts with surrounding rock matrix and the fluid it contains. The resulting weak problem is nonlinear, elliptic and symmetric, and can be given the structure of a fixed-point problem. For numerical simulations, we combine a XFEM discretization for the rock matrix deformation and pore pressure problem with a standard finite element method on a lower-dimensional grid for the fracture flow problem. The resulting coupled discrete problem consists of linear subdomain problems coupled by nonlinear coupling conditions. We solve the coupled system using a substructuring solver and observe very fast convergence. We also observe optimal mesh dependence of the discretization errors even in the presence of crack tips.

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Development of a Portable Lattice Boltzmann Code for Direct Numerical Simulations of Multiphase Flow in Porous Media and Microfluidic Devices

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The lattice Boltzmann method (LBM) has become a widely-used method to study multiphase flow in porous media and microfluidic devices, due to its ability to model complex interfacial dynamics and flow with complex geometry. Furthermore, the LBM is relatively easy to implement and is suitable for modern parallel computing, which is a requirement for simulations of flow in three-dimensional porous media due to the complex pore space morphology and the need to use large domains. For the past decade, many CUDA LBM codes have been developed to utilize Nvidia GPU acceleration. In recent years, many-core processors, such as the Intel MIC processor, have also been widely adopted in high performance computing. Due to the rapid development of modern processors, low-level CUDA code may not be a good choice for maintaining a portable code. As modern compilers become more and more mature, portable code using hybrid MPI-OpenMP or MPI-OpenACC, which relies on the compiler for low level implementation, could be quite attractive as one may run the same code on different platforms from every day laptop to high-end supercomputer equipped with GPU or MIC.

In this talk, we will introduce our experiences on optimizing our multiphase MRT-LBM code and porting the code to MIC and GPU via hybrid MPI-OpenMP/OpenACC programing. We adopt the AA pattern streaming method (Bailey et al., 2009) to reduce memory access and memory consumption, and the structure of arrays (SoA) data format to maximize vectorization. The bounce-back boundary condition is implicitly carried out by the AA pattern streaming method, and branching is avoided. Data communication is overlapped with data packing and inner nodes computation in order to improve parallel performance. We will present code performance results obtained from CPU, MIC and GPU, including the latest generation processors such as the Intel Knights Landing (KNL) processor. Significant speedup is observed even on CPU platform after optimization. Code performance on a KNL node is about 4 times the performance of an optimized code on a traditional CPU node with two 14-cores high-end CPUs. We will also present multiphase flow simulation results of our code on a real Bentheimer sandstone and a heterogeneous micromodel.

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Field emulators for a finite element porous media flow field simulator

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In this paper we develop field emulators for a finite element porous media flow field simulator with a random permeability field. We predict the velocity and pressure fields with high resolution, from which scalar summaries of the output can be extracted using quadrature rules.

The challenges fall into two categories: the high dimensionality of the input space (describing the permeability field) and the high dimensionality of the output space (pressure/velocity values at the FE nodes assuming a nodal basis). Two approaches are taken: a data-driven approach based on Gaussian processes and a Galerkin finite element reduced order model.

For the first we employ a KL expansion for the input and manifold learning to reduce the dimension of the output space, that is we locate a manifold on which the high dimensional outputs (vectorised pressure/velocity values at the FE nodes) reside and find an inverse map from the reduced dimensional coordinates to the physical space.

In a second approach we employ a KL expansion for the input space and use proper orthogonal decomposition to reduce the output space dimension. The snapshots for new input values are learned using high-dimensional output emulation based on manifold learning, as described above. This the approach is ideal for uncertainty quantification. We also investigate the use of generalised polynomial chaos expansions as an alternative to KL decomposition.

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Flow in weakly permeable porous media: a hybrid computational approach to determine effective properties

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Computational flow modeling and upscaling from pore scale to core scale has become a standard procedure in the last couple of years. Our recent contributions include an upscaling methodology applicable to large flow rates and anisotropy [1, 2], with pore geometries obtained from X-ray computed microtomography (micro-CT). We were also able to validate our computations with experimentally found permeabilities [3].

The micro-CT geometries are typically provided as binary data, i.e., a collection of voxels assigned either to the rock (impermeable) phase, or to the void phase (fluid in pores). A typical REV over which we compute and upscale corresponds to O(10M-50M) cells. The challenge in this paper is that many parts of the “rock” domain, after closer inspection, are also (weakly) permeable, but this feature is practically impossible to handle with the same micro-CT resolution, or, in contrast, with the flow simulations simultaneously accounting for the micropores and macropores. The closer inspection which motivates this study is from (a) a gap between the porosities measured at the CT-resolution and those from additional laboratory measurements. Further, (b) the realistic micro-pore matrix permeability is evaluated based on analysis of Scanning Electron Microscopy images.

The mathematical models of flow in the micro- and macro-pore domains use (i) the Stokes in macropores and Darcy in micropore domain coupled by the complex interface conditions (see [4] on vuggy media), or (ii) Brinkman flow equation [5]. We consider the third approach in which we systematically study the flow in the combined micro- and macro- pore domains with the same monolithic Direct Numerical Simulations solver; we present comparison with the results of (i) and (ii).

As an application we study isolation properties of weakly permeable mixtures of sand and clay. Such mixtures are used as components of sealing barriers in landfills’ construction. The samples of sand and clay mixtures contain from 100% to 20% of sand. Samples containing 80% sand or less are characterized by a low porosity detected at the micro-CT resolution, and some samples lack percolation.

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Impact of boundary conditions on the assessment of two-phase relative permeabilities from pore-scale numerical simulations

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We develop a numerical procedure conducive to the enucleation of the strength of capillary end effects impacting relative permeability estimates based on pore-scale numerical simulations of steady-state two-phase flow in three-dimensional reconstructed porous media. Accurate assessment of such relative permeabilities is a key challenge to modern characterization of subsurface flows in reservoirs/aquifers. In this context, the increasing availability of high resolution tomographic images of the complex pore space associated with rock samples should be matched by the development of improved numerical tools and simulation procedures yielding pore-scale distributions of state variables governing multiphase relative permeabilities. Here, we focus on a two-phase fluid flow setting mimicking steady-state protocols employed for relative permeability laboratory-scale experiments. Co-injection of a wetting (water) and a non-wetting (oil) phase is simulated at the pore-scale through a finite volume-based solver. The flow field is calculated within three-dimensional pore-spaces which are randomly generated via the procedure described in Hyman and Winter [1]. Our key objective is to assess the strength of the effects boundary conditions, i.e., capillary end effects, on the resulting relative permeability curves. We do so by considering porous micro-structures characterized by three diverse average pore size (hereafter termed as setting A, B, and C, respectively denoting systems with increasing average pore size) and length parallel to mean flow direction and illustrate the results associated with a given porosity (i.e., Phi = 0.48) and operating capillary number (i.e., Ca = 1e-3). Our results consistently show the establishment of three regions along the medium: (a) an inlet-disturbed (ID) region characterized by oil saturations which are relatively high and mainly driven by the inlet boundary value; (b) a bulk-undisturbed (BU) region where oil saturation appears to oscillate around a constant value; and (c) an outlet-disturbed (OD) region in which a sudden drop in oil saturation is observed. Capillary end effects drive the system behavior in the disturbed regions. Our results document that varying the length of the porous micro-structures along the main flow direction does not alter significantly the size of the disturbed regions. Thus, a bulk-undisturbed region is not clearly visible for the smallest pore domains. Considering diverse control volumes, i.e. including or excluding the disturbed regions, we conclude that estimates of oil relative permeabilities can be significantly biased toward low values if the disturbed regions are included in the calculation. Our procedure enables us to clearly identify the occurrence of capillary end effects and filter these from the estimated relative permeabilities grounded on our pore-scale simulations.

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Implementing Structured Mesh Vorticity-based Upscaling in Dual Mesh Method Reservoir Simulation

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Reservoir simulation can become a highly time and memory consuming procedure when considering high levels of heterogeneous geological systems. When looking at detailed geological data that produces refined grid-mesh used for solving pressure and saturation equations, the cost of reservoir simulation can reach unmanageable situation leading to degradation of the initial information. Based on this grand, an upscaled mesh is generated for the procedure in order to decrease time of calculation and keep the numerical error in a desirable range. A novel approach to upscaled detailed (fine) reservoir simulation from geological information is presented. Usually, upscaling procedures consist in generating a coarse mesh with an arbitrary method for dividing the number of cells in the three direction of a structured grid, and assigning an averaged effective permeability to the coarse-grid block which may generate both numerical dispersion and homogenization errors to be evaluated. In this paper, implicit-pressure explicit-saturation (IMPES) scheme is considered. Therefore it is predictable that homogenization error would have a major impact on the accuracy of the coarse-grid solution of the pressure equation. In order to reduce the homogenization error, we employ vorticity-based upscaling method which generates a non-uniform coarse grid with high resolution at high vorticity zones. Moreover, dual mesh method (DMM) is implemented to control the numerical dispersion error. DMM employs two different grids for solution of pressure and saturation equations. In this method, the coarse grid generated from vorticity-based upscaling method is used for solution of pressure equation, and the reference fine grid is used for updating saturation explicitly keeping the fine detailed data coming from the geological static models. The novelty of the method is the incorporation of the dual mesh method with non-uniform structural grid generated by vorticity-based upscaling method. This method improves the precisions of reservoir simulations using an accurate upscaled grid, and reducing the computational demand at the same time. To evaluate the method, we run two-phase simulation using SPE10 test case model 2. The obtained results indicate the good performance improvement provided by such an innovative approach.

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Influence of Interfracture Wave Induced Fluid Flow on the Seismic Wave Propagation

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Seismic wave attenuation due to fluid flow in porous media is, nowadays, one of the intensively studied effects because it may open a possibility to directly estimate reservoir capacity and permeability. It is moreover important for carbonate reservoirs where the fluid transport is supported by the system of fractures, filled with highly permeable material. Recently, numerical upscaling techniques based on quasi-static poroelastic equations [1] have become a popular tool for estimating attenuation caused by pressure diffusion effects in fractured media. In particular, in [2] the authors showed that two main mechanisms can be distinguished one caused by fracture-to-background flow, and one due to fracture-to-fracture flow, which essentially depends on the fracture connectivity. However, quasi-static upscaling does not account for the dynamic effects of wave propagation, in particular scattering. In this work we study the possibility to distinguish the interfracture fluid flow effects from scattering. We also verify that the attenuation behavior caused by pressure diffusion phenomena is equivalent for both approaches. Then we proceed to investigate the influence of dynamic effects on wave-induced fracture-to-fracture flow. The considered numerical model consists of a fluid-saturated porous medium containing randomly distributed vertical and horizontal fractures. In order to avoid scattering attenuation and to limit the frequency range in the wave propagation modelling, we study the various aspects of the diffusion mechanisms by varying the fracture permeability over several orders-of-magnitude. Overall, the two approaches show a good agreement (Figure 1), which confirms the adequacy of quasi-static upscaling procedures for scenarios where dynamic effects are expected to be negligible.

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InPore: Image-based Computational Pore-Scale Porous Media Flows

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Porous media flows are of significant interest in nature, science, and engineering applications. A few examples include the propagation of chemical contaminants in underground reservoirs, ink permeation, sedimentation, storage of hazardous wastes, and flow in oil reservoirs and biological tissues. Conventionally, due to the lack of appropriate research tools, porous media flow meant spatially and temporally averaged flow solved by phenomenologically and empirically derived constitutive equations such as Darcy's law, which results in difficulties to account for heterogeneity, complex pore inter-connectivity, and morphologies of porous media. In recent years, pore-scale porous media flow (PSPMF) has attracted increasing attentions by utilizing newly developed radiological imaging techniques such as computed tomography (CT), nuclear magnetic resonance spectroscopy (NMR), and magnetic resonance imaging (MRI); thus the celebrated Navier-Stokes (NS) equations have become the governing equations for porous media flows in pore space. However, there exist three major challenges that prevent general uses from powerful CFD for research: (1)steep CFD learning curve; (2) inability to utilize a series of existing software for pore structure extraction, geometry formation, and mesh generation; (3) demands of high-performance computation.

We develop a unique and easy access computational method [1] for imaged-based CFD. It's application, named InPore, for PSPMFs based on radiological imaging data to overcome the challenges. The features of InPore include (1) integrated modeling concept wrapping image extraction and fluid dynamics using mesoscopic lattice Boltzmann method(LBM) thus eliminating extra grid and mesh generation or data transfer involving a series of software packages; (2) local and fast computation via cutting-edge GPU (Graphic Processing Unit) paralleling computing technology thus no remote super computing resources are required for most applications. The LBM first solves a level set equation for image segmentation[2] and then extract the geometry and boundary information of the pore structure. The obtained pore structure expressed by volumetric ratio of solid versus fluid together with the orientation of local pore boundaries are seamlessly fed to volumetric LBM[3] that was specifically developed for solving fluid dynamics in arbitrarily complex geometries. Thanks to its inherent local data access in the collision-streaming stencils, the LBM is ideally amenable for parallelization over SIMD (single instruction, multiple data) architectures of GPU[4,5]. (3) grid upscaling to achieve large size, i.e., up to 2048^3, PSPMFs. We present an application study of natural gas/crude oil pore-scale flows in a digitized rock based on CT scanning image data. Focuses are on quantification of flow-rate and permeability in rockstones. The advantages and disadvantages of InPore are evaluated for solving PSPMFs for its further development.

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Numerical Simulation of Co-current Imbibition in Fractured Porous Media

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Water imbibition plays an important role in waterflood operations. The ultimate recovery primarily depends on the capillary forces that effect the immiscible displacement, where a non-wetting fluid is recovered from a porous reservoir rock by spontaneous imbibition of wetting fluid. This work presents numerical study of spontaneous imbibition process in a fractured matrix in two dimensional system and is based on immiscible two-phase fluid flow in fractured porous media. Complexity of immiscible two phase flow in two different media (matrix and fracture) and the interactions between the fluids, is the main reason behind using numerical models. Since the governing equations are coupled differential equations, there is no analytical solution for them. Therefore, numerical solutions such as finite difference and finite element methods through commercial software is considered. Various software programs can be used, but in our case the COMinisymposium OL Multiphysics has been found to be more favorable. Two phase Darcy law in the presence of capillary forces as well as relative permeability correlations in a porous media were adopted. Wetting and non-wetting fluids were considered to be water (Brine) and Crude Oil Respectively. Porous media was a core size matrix with a single fracture to mimic fractured oil reservoirs. Sensitivity analysis has been performed on various parameters such as matrix and fracture permeability, the angle between the fracture and matrix, fracture's width, and effect of gravity. The results indicate that regardless of fracture and matrix properties, a single fracture in a porous media can lead to a high acceleration in spontaneous imbibition flow and much lower breakthrough time in the same media without fracture.

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Optimization for grid strategy and time stepping strategy of multi-time scale simulation

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Modern information about subsurface reservoirs includes traditional data, coming from production scale measurements such as dynamic well rates, and transient scale information, such as dynamic pressure distribution from in-situ gauges. To take a full advantage of reservoir response at both scales, we designed a specific reservoir discretization framework which make simulation model sensitive to transient and production scale changes. We used a multi-segment well model to capture the effect of the multiphase flow in the wellbore including the influence of hydrostatic, friction, acceleration and drift-flux to the transient and production scale forecast. We developed an optimized strategy for the design of simulation model based on a fully unstructured 3D tetrahedral grid. Using the advanced gridding approach, we designed an optimized discretization in time to keep the sensitivity to both type of information. We applied the designed framework for the reconstruction of major reservoir features in the section model of CO2 injection for EOR.

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Quantification of tortuosity in Molecular Dynamics models using Nernst-Einstein relation

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Porous materials, such as rocks, polymers, glasses or composites, find numerous applications due to their outstanding mechanical properties, specific weight, and thermal conductivity. The molecular dynamics (MD) simulations, due to their versatility, as well as satisfactory temporal and spatial resolution, are a convenient tool for the investigation of atom-scale physical phenomena, such as gas transport in a porous structure. We present here a novel numerical method to estimate the pore network tortuosity that does not require any dynamical simulation and is based only on given MD structure. The applied methodology allows for quantification of the pore network of an MD system by determining: total porosity, 'isolated' porosity, surface area of the pores and well as their size distribution. Moreover, we provide the numerical path to obtain the diameter distribution from the (commonly used) chord distribution that, as we demonstrate, always overrepresents smaller pores. For the first time the analysis of MD simulation can be enhanced by the tortuosity analysis that does not require extensive MD simulations, using instead directly obtained pore structure of an MD system. The conductivity of the pore system is estimated based on the Nernst-Einstein equation. The determination of geometric-based conductivity can be immediately linked to tortuosity of the porous system without the requirement of diffusion calculation. We apply this methodology to the case of swelling pore system of two hydrophilic polymers: amorphous cellulose and amorphous hemicellulose. The two systems display the same response of increasing hydration: the pore network, evolving with the concentration of adsorbed water, expands due to pore merging and increase of their size. This phenomenon, together with the de-entanglement of polymer chains, results in a decrease of tortuosity and explains the non-linear diffusion coefficient in many porous materials, such as wood.

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Simulating the dynamics of chlorinated NAPL source zone remediation in porous media during the injection of nZVI suspensions

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Nanoscale zero-valent iron (nZVI) is currently used widely for the in situ remediation of aquifers from a variety of toxic pollutants (e.g. reduction of chlorinated hydrocarbons, and nitro-aromatics, sorption/geochemical trapping of heavy metals/metalloids) (Mueller et al., 2012). The macroscopic modeling of nanoparticle transport during their injection in porous media is of key importance for the interpretation of lab-scale tests and design of efficient field-scale applications (Tosco et al., 2014; Tsakiroglou et al., 2016). Although extensive work has been done on the simulation of nZVI transport and immobilized nZVI interactions with NAPL and dissolved species, there is a lack of numerical models coupling the multiphase transport with reactive processes during the continuous injection of nZVI in porous media partly saturated by trapped NAPL (chlorinated hydrocarbons) ganglia. In the present work, such a macroscopic numerical model of reactive nZVI flow in porous media is developed by using the software platform of ATHENA Visual Studio. First, the nZVI transport in porous media is simulated by using the model of Tosco et al., (2014). The numerical code is used to perform a sensitivity analysis, and elucidate the effects of process dimensionless parameters (Peclet number, Dimensionless flow velocity, Damköhler number for particle deposition) on the nZVI concentration breakthrough curve (Fig.1). Inverse modeling of experimental results from tests performed on a glass-etched pore network, enables us to estimate the parameters describing the kinetics of nanoparticle attachment / detachment. Second, a statistical shrinking-core model that couples the mass-transfer with reactive processes at the nanoparticle scale, along with experimental results from batch tests of tetrachloro-ethylene (PCE) dechlorination by nZVI (Tsakiroglou et al., 2015) enables us to develop an analytic phenomenological model providing the overall reaction rate as a function of PCE and nZVI concentrations. Then, the macroscopic nZVI transport model is extended to reactive flows by including (1) mass balances for residual NAPL saturation (source zone), and dissolved pollutant concentration (aqueous phase), and (2) phenomenological models quantifying the dynamics of PCE dissolution and nZVI reactivity. A sensitivity analysis is performed with the aid of extended model to clarify the effects of dimensionless parameters (Sherwood number, Dimensionless flow velocity, Damköhler number for reactions) on remediation efficiency (Fig.2). The model is evaluated with respect to its capability to predict experiments of nZVI injection in a glass-etched pore network (Fig.3) and a soil column, both partially saturated with trapped ganglia of tetrachloro-ethylene (PCE).

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Simulations of Reactive Transport in Technical Porous Media: Dealing with Heterogeneities and Examples From Catalytic Filters

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Introduction Reactive flows in porous media are an important process in many industrial and environmental applications. The reactive transport in porous media is influenced by the interplay between convection, diffusion and reaction, coupled with the heterogeneity of the pore space (e.g., pore size distribution and connectivity) and chemical heterogeneity (e.g., polymineral rocks). Understanding these processes and their dependence on chemical and morphological parameters poses a number of research challenges. In this talk we will shortly present a recently developed software tool for simulation of reactive transport, PoreChem, and will show results of simulations for recent applications of reactive flow in porous media, ranging from geoscience to catalytic filters.

Pore-Scale Simulation To perform the simulations Fraunhofer ITWM has developed PoreChem [1,2,3], a software package dedicated to the simulation of reactive flow on the pore-scale. It enables the simulation of reactive flows in resolved porous media in a reasonable time. The software can compute the flow of a fluid in the pore space, as well as the diffusive and advective transport of a solute species. Reactions can then be simulated occurring not only in the fluid volume but also on the surface of the porous medium and on interfaces between two fluid phase regions. The flow is computed by solving the Navier-Stokes-Brinkman system of equations with a finite volume discretization on a regular voxel grid. Transport and reactions are simulated by solving the reaction-diffusion-advection equation with the same discretization coupled to the surface concentration by Robin boundary conditions. For the reactions, different reaction kinetics, parametrized by reaction isotherms can be taken into account. The fast voxel based solver enables calculations directly on µCT-Images. Transient phenomena can be simulated, as well as steady states ones.

Results To illustrate the modeling and simulation, we show results of numerical studies in the field of catalytic filters. Here the filtration process takes place in a two scale porous medium. The reaction occurs in nanoporous particles, where the pore space is not resolved, but is taken into account as a volumetric sink. We show the computation of filter efficiencies on segmented 3D CT images using PoreChem at the microscale. Furthermore, we show results from computations at the macro scale using the commercial software tool COMinisymposium OL, where the parameters for the homogenized model are calculated from the solution of cell problems at microscale. Results from microscale and macroscale solutions are compared.

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Space-time grid adaptation for solute transport in heterogeneous porous media.

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We assess the impact of adaptive anisotropic space and time discretization on our ability to accurately model solute transport of non-reactive chemicals in heterogeneous porous media through the Advection Dispersion Equation. Heterogeneity is characterized in terms of the spatial distribution of trasmissivity, whose natural logarithm, Y, is treated as a second-order stationary random process. An advective steady-state velocity field is considered, as rendered by the solution of Darcy's Law and standard mass conservation. A suitable recovery-based error estimator drives the adaptive discretization. We investigate two diverse strategies guiding the anisotropic meshes adaptation. The error estimator of each of these is assessed on the basis of spatial gradients of (i) only solute concentration, or (ii) both concentration and velocity components. We test the methodologies for two-dimensional synthetic cases with moderate, an high, level of heterogeneity, being the variance of Y. As quantities of interest against which to assess the accuracy and efficiency of our approach, we focus on the time evolution of section-averaged and point-wise breakthrough curves, second centered spatial moment of the advancing solute plume and the scalar dissipation rate associated with the concentration field. We find a satisfactory comparison between results for the adaptive methodologies and reference solutions associated with fixed space-time discretization, whose degree of resolution is assessed on the basis of a convergence study. Comparison of the two adaptive strategies highlights that: (i) defining the error estimator only in terms of gradients of concentrations leads to some advantages in characterizing solute transport in correspondence of low velocity regions, where diffusion-dispersion mechanism dominate; (ii) incorporating the velocity field in the guiding error estimator leads to improved characterization of the advancing front of the migrating solute which propagates through high velocity channels.

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A new application of NMR in characterization of multi-phase methane gases and adsorption capacity of shale

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Different from typical conventional reservoir rocks such as clastic and carbonate rocks, gas shale has large amount of nanopores, within which multi-phase of gases can exist. It is well known that the internal interaction mechanism of multi-phase gases in reservoirs is extremely important for accumulation and production of shale gas. However, to the best of the authors' knowledge, there is not a systemic investigation of this topic in exist literatures. As a kind of new 1H probe technology, NMR relaxation time analysis provides a method of pore structure analysis for porous medium, and enables studies of the transportation of hydrogen-containing fluids in gas shales. When a low magnetic field was used for a NMR measurement, the signal of mobile hydrogen nucleus or proton in methane can be detected, whereas the signal from solid 1H in organic matters of shale cannot detected due to extremely fast relaxation. Thus, the 1H probe technology has potential to be used in characterization of multi-phase gases in the nano-pores of gas shales. In this study, several special experimental setups were designed and used to evaluate the adsorption of multiphase methane gases in shales. By introducing the low-field NMR into the gas shale reservoir, we firstly developed several models and methodology, including 1) a methodology for quantitative identification of multi-phase (adsorbed-, porous-medium-confined-, inter particle bulk-, and bulk) methane gases in shales, 2) a theory and analytical technique to determine the methane isothermal adsorption capacity of shales. Then two limitations of the use of this method are 1) avoiding an inhomogeneous field effect resulted by ferromagnetic mineral composition in shales; and 2) eliminating the influences from diffusional exchange of fluid in micropores and macropores. As a conclusion, we suggest that the developed 1H probe technology can be applied as a noninvasive analytical technique to characterize the multi-phase gases in the nano-pores, and has great potential in enhanced gas recovery (EGR) and Carbon Capture Utilization and Storage (CCUS).

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Biomineralization: a strategy to modify permeability in the subsurface

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Strategies to mitigate leakage pathways or seal fractures in the subsurface are important to seal leaking wells or control fluid transport. Biomineralization is a proposed technology for sealing unwanted leakage pathways in the near wellbore environment and modifying permeability in the subsurface. The biomineralization sealing technology developed at Montana State University utilizes microbes to promote biomineral formation in fractures (for example fractured shale, sandstone, or between cement/steel interfaces) and in the pore spaces of rocks (for example sandstone).

Reactor systems have been designed in the laboratory to study the permeability reduction achievable by biomineralization under ambient and subsurface pressure conditions. These reactor systems are being used to develop injection strategies which have resulted in 3-6 orders of magnitude permeability reduction in 100 µm- 4mm gaps between shale, sandstone and cement/steel interfaces. The laboratory reactor systems were used to scale up and develop injection strategies applicable to the field. Reactive transport modeling has been performed at the University of Stuttgart to enhance the design and support the success of the laboratory and field experiments.

Two field demonstrations of the biomineralization sealing technology have been completed [1]. The first demonstration showed fracture sealing was possible in a sandstone formation 341m below ground surface and that the fracture had increased resistance to re-fracturing after biomineralization treatment (Figure 1). The second field demonstration was performed in a well with an identified channel 310m below ground surface in cement near the wellbore. Biomineralization treatment resulted in reduced pressure decay during shut in periods and reduced injectivity. In addition, a noticeable difference was observed in the solids percentage in the ultrasonic imaging logs before and after biomineralization treatment. These successful experiments suggest biomineralization is a promising technology for modifying permeability in the subsurface. Work continues to develop strategies to promote mineralization in CO2-affected brine environments as well as in high temperature environments.

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CO2 TRAPPING AND GEOELECTRICAL CHARACTERISATION OF GEOLOGICAL CARBON SEQUESTRATION

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Carbon sequestration is a promising method for reducing carbon dioxide (CO2) emissions as it permits the storage of compressed CO2 in the subsurface. The carbon sequestration sites must be monitored in order to detect potential leaks; one way of which being the monitoring of geoelectrical properties such as electrical conductivity (σ) and dielectric constant (ε). This investigation focuses on using Time Domain Reflectometry (TDR) probes to determine the influence of different factors on the measurements of the electrical conductivity (σ) and dielectric constant (ε) of a porous rock reservoir in relation to the soil water saturation (Sw). The factors investigated were salt concentration, pH, rock type and presence of surfactant which are unique to a given storage site. This was done via a number of dynamic two-phase flow experiments using gaseous CO2. It was found that salt concentration, rock type and presence of a surfactant had a significant effect on the σ-Sw and ε-Sw relationships. Higher salt concentrations were found to give higher values for σ and ε for given Sw values. Limestone was found to give the highest values of both σ and ε for any given Sw, followed by silica and basalt. The presence of a surfactant resulted in higher values for σ at higher Sw values and lower values for σ at lower Sw values compared to when no surfactant was present. Surfactant presence also resulted in lower values for ε at given Sw values. Initial pH values (with Silica sand) were found to have no significant effect on the σ-Sw and ε -Sw relationships. The applicability of mathematical models to the results obtained was investigated. The reliability of the measurements of σ and ε indicate that the use of TDR presents a viable monitoring option.

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Colloid deposition in monolithic porous ceramics - experimental investigations using µCT and MRI

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The transport and deposition of colloids within porous media plays an important role in numerous natural and technological processes, such as oil extraction, water treatment and subsurface contaminant transport among others [1-3]. In a technological context the process itself is denoted as deep bed filtration. In the last decades, model systems of porous filter structures (e.g. packed beds of glass beads) were a major subject of research (e.g. [2-4]). However, monolithic filters like sponges have not been studied extensively until now. Therefore, it is the aim of this work to investigate deep bed filtration processes in monolithic porous ceramics [5].

The mechanisms of colloid deposition are known in principle [6]. However, only macroscopic information about deep bed filtration processes is usually available. In this work a novel experimental approach has been chosen to investigate deep bed filtration processes on a microscopic scale. To this end, two imaging modalities, Micro-Computed X-ray Tomography (µCT) and Magnetic Resonance Velocimetry (MRV), have been applied. While µCT offers topological information of the filter (pore structure, porosity, etc.) as well as the spatial distribution of immobilized colloids, MRV provides the three-dimensional velocity fields of the liquid within the filter. With the combination of both techniques the influence of the velocity fields on colloid deposition will be evaluated (see fig. 1).

The experimental studies were carried out as follows. The clean filter was placed in a customized flow cell which was then mounted in a 7-Tesla MRI (Magnetic Resonance Imaging) scanner and subsequently rinsed with distilled water at a constant flow rate. Afterwards, the flow cell was moved to a µCT scanner in order to perform deep bed filtration experiments. Therefore, a diluted suspension consisting of distilled water and tin oxide particles was pumped through the filter with the same flow rate that was used before. Eventually, a series of µCT scans was performed in order to image the temporal evolution of particle deposition sites within the filter. First results indicate a relation between the local velocity magnitude and local concentration of deposited particles. On the one hand an increased velocity corresponds to an increased influx of colloids while on the other hand increased shear forces are unfavorable for the deposition of colloids. It can be shown that particles tend to accumulate in regions with lower fluid velocities (see fig. 2).

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Compression and erosion resistance properties of foam concrete

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To analyze the compression properties and erosion resistance properties of foam concrete used in geotechniacal engineering, one dimensional compression tests were carried out using ring specimens of foam concrete, and unconfined compression tests were carried out using foam concrete specimens cured in different conditions. The results of one dimensional compression tests show that the compression curve of foam concrete has two critical points and three stages, which has significant difference with ordinary geotechnical materials such as soil. Based on the compression curve the compression modulus of each stage was determined. The results of erosion tests show that sea water has a slight influence on the long-term strength of foam concrete, while the sulfate solution has a significant influence on the long-term strength of foam concrete, which needs to pay more attention.

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Development of a ratiometric method to measure viscosity inside mesoporous silica particles using protein-bound fluorescent probe

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Mesoporous silica particles are used for immobilization of enzymes in order to increase enzyme stability, facilitate product purification and reuse of enzyme. Many efforts have been done to investigate how the environment inside the pores changes after enzyme immobilization and how it can affect activity and stability of immobilized enzymes. One of these environmental changes can be viscosity inside the pores and comparing the difference with the bulk solution. Here, we investigate viscosity inside mesoporous silica particles, SBA-15, 1µm diameter with 9nm pore diameter, based on two different cyanine fluorophores which are sensitive to viscosity, Cy3 and Cy5 using a ratiometric method. The probes can bond covalently to lipase as enzyme used in two different conditions: a. both probes seated on one enzyme, b. they can be attached to the enzyme separately. We work with a ratiometric method to measure only viscosity and no other solvent effects. In this study, Cy5 can be used to normalize for polarity other than viscosity. In addition, we take advantage of the energy transfer (FRET) between probes when they are seated on one enzyme and measure the distance between them.

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Development of Silica Gel Nanoparticles for Inhibiting the Precipitation/Deposition of Asphaltenes

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Asphaltenes are the heaviest fraction of crude oil, mainly structured by a poly-aromatic core linked to alkyl chains containing compounds as sulfides, nitrogen and oxygen and metals including vanadium, iron and nickel [1, 2]. Due to its high polarity, aggregation ability and subsequent precipitation/deposition can cause various problems such as altering the wettability, pore blocking and permeability/porosity reduction. Therefore, the objective of this work is to evaluate the effect of the particle size, surface area and surface acidity of silica nanoparticles on the inhibition of formation damage caused by asphaltenes. Silica gel nanoparticles were synthesized through the sol-gel method, and their characterization was performed via N2 physisorption at -196°C, field emission scanning electron microscopy (FESEM), dynamic light scattering (DLS) [3] measurements and NH3 temperature programmed desorption (TPD) [4]. The ability of the nanoparticles to adsorb asphaltenes and to reduce asphaltene self-association was evaluated using batch-mode experiments. The kinetics of asphaltene aggregate growth in the presence and absence of nanoparticles were evaluated using DLS measurements in different heptol (n-heptane/toluene ratio) solutions [5]. Indeed, nanoparticles with lower average particle size, higher surface area and higher total acidity: S11, had higher adsorptive capacity between the materials studied. In general, the synthesized nanoparticles successfully reduced asphaltenes aggregation and subsequent precipitation/deposition through the adsorption of these compounds on the nanoparticles. Silica nanoparticles exhibit high thermal and chemical stability, making them conducive to in-situ application. Additionally, in this study, the performance of a nanofluid treatment was tested under flow conditions in porous media under typical reservoir conditions using the nanoparticles with the best performance in batch-mode experiments. Indeed, nanofluid treatment with silica nanoparticles increased the effective permeability to oil and enhanced the oil recovery with an increase in the recovery factor of 11% under the conditions reported here [6, 7]. The use of nanoparticles is a promising technology for the inhibition and control of different types of formation damage as asphaltene deposition at the reservoir because it has a high cost/benefit ratio compared with other conventional treatments. It is worth noting, the use of this technology for inhibiting formation damage by asphaltenes has a significant effect on wettability alteration, which in turn increases the mobility of the oil and promotes productivity of reservoir.

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EFFECT OF CHEMICAL NATURE OF FINES AND NANOPARTICLES ON THE INHIBITION OF FORMATION DAMAGE CAUSED BY FINES MIGRATION

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The migration of fines is one of the principal problems in the production phases of the oil wells, this migration causes plugging of throats in porous media, affecting the permeability of reservoir declining the productivity and injectivity. In different studies of the production of oil well has been encounter evidence the high decline in productivity as a result of a reduction in permeability near the wellbore a consequence from an accumulation of fines. In general, the migration of fines is a damage associated to the mobilization of fines particles and their accumulation in throat pores. The fines restrict the flowing of fluids due to the size of the pore is smaller than the particle or in cases when various particles very fines treat to cross the throat pore at a time, resulting in bridging and sedimentation of them. Several authors have proposed different techniques to solve the problem, but these solutions present some problems and disadvantage in its application. Therefore the nanotechnology emerges as an important tool to address various challenges. The nanoparticles (size less 100 nm) allows combining the extremely high surface area with high adsorptive capacity, acting effectively in the fixation of formation fines and stabilization of the interaction forces. Nanofluids that contain nanoparticles show specific properties such as the high tendency for adsorption which make a good option for the injection into the near wellbore regions because of their very small sizes [1-3]. In different studies is mentioned the use of nanoparticles, however, is not report studies about the evaluation of effect of the chemical nature of the fines and its influence in the inhibition ability of nanoparticles of a different type. Thus, this is the objective of this work. On this way, in this work experimentally was modeled the adsorption system of package sands beds, through which flowed the fines suspension. The adsorbent sand beds were prepared with Ottawa sand (12-20 and 25-40 mesh). Two different packed beds were used in this study: clean sand (simulating the water wettability) and sand submitted to a damaging process using an extra heavy crude oil (wet oil condition). These packed beds were treated with nanoparticles of iron oxide, silica, and alumina. The suspension of fines was prepared with quartz, kaolinite, illite and its combination in different proportions to show the effect of the fines chemical nature. The Adams-Bohart, Clark, and Wolborska models were used to fit the experimental data of rupture curve. For this purpose, a three components Simplex-Centroid Mixture Design (SCMD) is employed by evaluating seven points at different concentrations for each element to adjust the response variable for the design and the desired model. The response variable depends on the model and can be: mass transfer coefficient or capacity adsorption of the medium.

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EFFECT OF TYPE OF PROCESS CONTROL AGENT ON THE SYNTHESIS AND CHARACTERIZATION OF Cu25W COMPOSITE POWDER

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This study investigated the effect of various process control agents (PCA) on the synthesis of Cu25W composite powder. The usage of PCAs is crucial to avoid agglomeration and to decrease the tendency of cold welding among powder particles. Hence, two different types of PCA, namely stearic acid and polyethylene glycol (PEG) were added separately to powder mixtures containing elemental copper (Cu) and tungsten (W) powders. Then these mixtures were filled in vials of a two stationary planetary-type ball mill. Ball milling parameters, namely ball-to-powder weight ratio and milling speed were selected 10:1 and 300 rpm, respectively [1]. Characterization of the milled powders was evaluated as a function of type of PCA and milling duration using scanning electron microscopy (SEM) and laser diffraction analysis (Mastersizer). As a result of this effort, it was observed that the variation occurred in both morphology and final powder particle sizes depending on the type of PCA. In addition, stearic acid was found to be more effective as compared to PEG in terms of achieving particle size reduction (Fig. 1).

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Experimental Investigation of Hysteretic Dynamic Capillarity Effect in Unsaturated Flow

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Capillary pressure, defined as the difference in fluid pressures, is commonly assumed only to be a function of saturation. However, rate dependency in capillary pressure-saturation relationship under transient flow has been observed over decades. Among others, a dynamic term depending on the changing rate of saturation, referred to as dynamic capillarity effect, is widely used to explain this phenomenon. In this study, a series of laboratory experiments was carried out to quantify the dynamic capillarity effect in an unsaturated soil. Both static and dynamic primary, main and scanning drainage experiments were performed in a small-volume sand cell with highly characterized water sensors. The value of the dynamic capillarity coefficient τ was calculated based on local pressure difference and average saturation measurements during static and dynamic drainage experiments. A similar trend of the dependence between τ and saturation was found for primary and main drainage. As the saturation decreased within the saturation from 0.9 to 0.4, its value decreased slightly at first, then varied little for the moderate saturation range, and increased nearly linearly afterwards. While the value of τ increased for scanning drainage, as the saturation decreased from 0.5 to 0.3. Nevertheless, the magnitude of τ for primary drainage was found to be larger than main drainage over the entire saturation range, while τ value was much smaller for scanning drainage. It implies that the relationship between τ and saturation is non-unique, i.e. hysteretic. Moreover, the value of τ in our study, ranging from 1.5*10^5 to 4*10^6 Pa·s, was consistent with those reported values.

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Experimental investigation of micro structures extension of the defects of coal semi-submitted by liquid nitrogen

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The coal bed is a typical porous media, and its permeability is a key issue for methane recovery and drainage. Injection of liquid nitrogen into low-permeability coal bed is a new technology of fracturing coal and improving permeability of coal. To investigate the micro structures extension characteristics of the defects of coal samples semi-submitted by liquid nitrogen, the experimental setup of coal sample semi-submitted by liquid nitrogen was made in this paper. The anthracitic coal was obtained from Shanxi province the standard samples with different saturation were handled. Then the semi-submission experiment in liquid nitrogen for the samples was performed. The non metallic ultrasonic tester was employed to measure the ultrasonic velocity before and after the action of liquid nitrogen. The photomicroscope was employed to investigate the cracks' width extension of coal samples before and after the action of liquid nitrogen. The results show (1) the saturation of coal samples has great effects on the cracks' extension subjected to liquid nitrogen. The ultrasonic velocity change and the cracks' width extension of the saturated coal samples are maximum, Those of the semi-saturation coal samples become worse. Those of dry coal samples are worst. (2) The nearer to the surface of the liquid nitrogen, the greater the temperature change of coal samples is. And there is much more significant effect of liquid nitrogen. (3) The main reason of the cracks' extension of the saturating and semi-saturation coal samples is the frost heave pressure caused by the phase from water to ice. Thermal stress due to temperature gradient induces the cracks' extension of dry coal samples.

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Experimental study of clogging of subsurface pores in the vicinity of dams in arid zones: groundwater recharge efficiency and potential solution

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Groundwater recharge dams represent one of few practical engineering techniques to augment the limited water resources. Formation of a low-permeable cake by deposition of suspended particles transported by ephemeral flashfloods is a common problem for dams in arid regions (e.g., Oman). The Al-Khoud dam, Oman, is considered in this study (Ebrahim et al., 2015). Accumulation of surface sediments impacts many hydrological properties of dam's reservoir area, including reduced infiltration and deep percolation rates, higher water loss via evaporation, and ultimately lower aquifer recharge. The recharge basin downstream the dam receives pulses of suspended sediments after each major flashflood. This causes a "hopping" downward translocation of fine particles into the coarse-texture matrix of the parent alluvium, clogging of the pores and hence reduces the saturated hydraulic conductivity (Ks) (Faber et al., 2015). Ks drops with depth from 3.9 cm/h at the surface to 0.37 cm/h at a depth of 80 cm (Al-Saqri et al., 2015). There is a remarkable difference with clogging of sand filters or gravel packs of production water/oil wells, which are continuously subject to Darcian hydraulic gradients, viz. heterogeneous, multilayered reservoir beds are at essentially intermittent, relatively short and transient impacts of flood-induced vertical infiltration gradients which "restructure" the soil profile. The non-monotonic curves of silt and sand contents are corroborated by infiltration tests and pore-scale models (Al-Maktoumi et al., 2015). The discovered "reversed" textural profiles and non-monotonic cumulative infiltration curves have intricate hydro-engineering implications, e.g. we observed that the runoff water, released from the dam, instead of a fast vertical infiltration, forms a shallow quasi-horizontal Darcian flow that out-seeps further downstream into local topographic depressions and contributes to undesired runoff-evaporation. A laboratory column-experiment to study the dynamics of vertically translocated particles (silt and very fine sand) was conducted using two course matrix skeletons: glass beads, and artificial sands (Faber et al., 2015). At the beginning, the top few centimeters got clogged by retained fine particles. The silt retention front continued to migrate downward until the top layers of the column attained full clogging and the front stopped descending. The Ks showed a sharp change at the interface below and above the silt retention front. It dropped by 30 and 50 % due to clogging for glass beads and artificial sand respectively. A hydro-ecological method of combatting the cake-clogging curse is vegetation (trees and shrubs growing in the reservoir area). In tank experiments (using 14 tanks), we quantified the effect of roots of indigenous trees (Sider and Ghaf Trees) on increasing infiltration through a clogged layer. Infiltration tests showed that the infiltration rates increased by 6 times in tanks with cultivated trees (10-14 mm/h at the initial stage in both control bare soil and planted tanks to around 62 mm/hr in the latter after 12 months of cultivation). Our results indicate the feasibility of the hydro-ecological techniques in improving the infiltration rate and hence the recharge efficiency of recharge dams in arid areas.

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Experimental Study of gas Flow Behavior in Tight Reservoir by Using Micro Tubes

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Due to the small pores and fine throats of the tight reservoir, collisions between gas molecules and pore walls increase greatly. For the similarity to that of rarefied gas flow, slip boundary condition that based on the rarefied gas theory was applied to modify the conventional Darcy theory in order to describe the non-Darcy flow of gas in tight reservoirs more precisely. In this study we attempted to explore if gas flowing in tight reservoir can be considered as rarefied gas flow under reservoir conditions. To that end we conducted micro tube flow experiment under in-situ pressure and temperature conditions to simulate gas flow in tight cores, eliminating the influence of multi-scale throats. Then we explored the impact of different end-pressure, differential pressure and gas type on flow behavior of gas in micro tubes. In addition, we presented corresponding gas apparent permeability of the equivalent cores. The results indicate that slip boundary condition will lead to errors when the end-pressure was higher than 8.3MPa in the micro tube with the inner diameter larger than 2μm. With increasing of end pressure, the flow behavior gradually coincided with Darcy's law. While along with the increase of differential pressure, the flow resistance raised dramatically, resulting in the deviation of apparent permeability curve down towards from the Klinkenberg curve. This phenomenon casts doubt on the rationality of frequently used slip boundary condition under reservoir conditions and has never been discussed previously by micro tube experiments. In order to find the basic law of gas flow in tight reservoirs, the nature of the flow generated by the tiny scale must be characterized under reservoir conditions. Our analysis showed that enhancing the average gas pressure for simulation of high pressure gas flow by increasing pressure difference doesn’t conform to the physical reservoir situation. What’s more, it tends to lead improper results.

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Experimental study of non-Darcy flow mechanism using micro-tubes under high pressure and verification of theoretical models

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Because of the effect of small pore throats, gas flow behaviors in tight reservoirs differ from that in conventional reservoirs greatly. Most of authors studied this phenomenon theoretically and ascribed such deviation from Darcy's law to slippage effect or Knudsen diffusion. Based on that the transport equations of gas in tight reservoirs has been improved. However, few investigations have been made by conducting experiments and most transport models remain to be experimentally verified. In this paper, we attempt to apply the experimental method to explore the flow characteristics of gas in tight reservoirs and test the applicability of theoretical models. First, we conducted gas flow experiments using micro circular tubes with different diameters to simulate gas flow in different throats of tight cores. And high pressure has been imposed on both end of the micro tube connector designed by ourselves to simulate the in-situ pressure. Then we explored the impact of different end-pressure, differential pressure and gas type on flow behavior of gas in micro tubes. In addition, accuracy of three whole-regime models, including the Beskok-Karniadakis model (Model A), a continuum flow & Knudsen diffusion combination model (Model B), and a slip flow & Knudsen diffusion combination flow model (Model C) has been compared based on the experimental results. The results imply that the dimension of the tube has a significant effect on gas flow characteristics. Under low pressure, the smaller tube radius, the higher deviation between the experimental results and the theoretical predictions of H-P theory which is the basis of permeability calculation . With increasing of end pressure, the flow behavior gradually coincided with the conventional theory. While along with the increase of differential pressure, the flow resistance raised dramatically. It is also evident that the influence of pressure became dominant in tubes with smaller radius. Comparing experimental results with theoretical perspectives, we found a good agreement between the Model C and experimental measurements in 2μm micro-tubes. With increasing diameter of micro-tubes, our measurements in 5μm and 10μm micro-tubes kept accordance with the Model B. However, at all situations, the numerical result of Model A was nearly the same as Model B's, 9~16% lower than measurements. Our research sheds some light on the mechanism of gas flow in micro scale pores. Most current theoretical models are based on rarefied gas theory, which is far from the environmental condition of gas underground. Our efforts contribute to modeling improvements of non-Darcy gas flow.

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Imaging of single and multi-phase flow in porous rocks with sub-resolution micro-pores using X-ray microtomography differential imaging

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Fluid flow in porous rocks plays an important role in many subsurface applications, such as reservoir engineering and subsurface hydrology. In recent years, there is a growing interest in using imaging technique to quantify and assess the flow and transport in porous rocks. This normally includes obtaining and computing flow related parameters, such as permeability, directly from image analysis. Characterisation of the pore space within the rocks is one of the most important steps. The understanding of the impact of the sub-resolution micro-pores remains challenging, and needs to be better explored. We present a new single phase experimental methodology that uses high-salinity contrast brine and differential imaging acquired by X-ray tomography to non-invasively obtain three-dimensional spatially resolved information on porosity and connectivity, including sub-resolution micro-porosity. This results in spatially resolved maps of the solid grain phase, sub-resolution micro-pores within the grains, and macro-pores. The total porosity values from the three phase segmentation for the selected rock samples are shown to be in good agreement with Helium porosity measurements.

We show how this experiment methodology can be further applied to study multi-phase flow in porous rocks. A drainage experiment with porous plate that injects nitrogen to displace brine in a sandstone is presented, in order to image and compute the brine distribution map at different capillary pressures. It can be observed that the brine started to be displaced in the macro pores at low capillary pressures, followed by the displacement in the sub-resolution pores at high capillary pressures. The average brine saturation values at different capillary pressures have also been quantified. Overall, the new method offers a capability to characterise a range of single and multi-phase flow and transport phenomena in porous rocks.

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INVESTIGATION OF PARTICLE SIZE EFFECT ON THE SYNTHESIS OF W-REINFORCED Cu-BASED COMPOSITE POWDER

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This study investigated the effect of particle size on the synthesis and characterization of Cu25W composite powder. For this aim, elemental copper (Cu) powders having two different particle sizes were separately mixed with tungsten (W) powders. A two stationary planetary-type ball mill was used to carry out milling experiments with a ball-to-powder weight ratio of 10:1 and a milling speed of 300 rpm [1]. Characterization of the milled powders was determined as a function of particle size and milling time using scanning electron microscopy (SEM) and laser diffraction analysis (Mastersizer). It was found that the size and shape of the starting powder particles significantly affect the rate of fracturing and the final powder particle size (Fig. 1).

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Laboratory evaluation of the performance of polymer nanocomposite gels in porous media and evaluate the rheological behaviour of water reservoirs in one of the Iranians reserviors

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Now stop the flow of water in producing wells is a major problem in petroleum engineering, so that account for a significant cost and production efficiency. Important an application of polymer nanocomposite gel (polymer reaction, a network operating a mechanism of nano particles) in the oil industry, production control water closing routes with high permeability. In this work, the effect of montmorillonite clay and network operating mechanism on the physical and chemical properties of chromium acetate polymer gel produced by xanthan polymers (because of high salinity of reservoir) has been studied. Example of various consistency of network operating mechanism and made clay of investigation on test shrinkage, evaporation rate, the percentage swelling and rheological test to determine the characteristics of the polymer system to prevent water from tensile tests have been performed in porous media. The results for all samples indicated that the evaporation rate is increased with increasing clay. The test results are wrinkles, reduce wrinkles is shown. Increasing latency and increase network operating mechanism, reduce the percentage of inflation. The results of rheological water injection and decreased permeability reduction in porous media shows. Also, due to the high cost of gel injected in porous media in the laboratory, can be rheological data and simulations of the polymer gel to ensure accuracy.

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Layer-By-Layer (LBL) surface modification of microfluidics with geo-materials: Towards subsurface porous media

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The properties of rock surfaces contribute significantly in physics of subsurface multiphase flows. Microfluidics technology with its great advantages for direct visualization and real-time observation has drawn booming attention in energy innovation and brought new opportunities on precious pore-scale studies [1, 2]. However, considering the restriction on present microfabrication materials and surface property control techniques, studies on many aspects relevant to rock-fluid interactions may not be fully developed in microfluidic systems. There is a pressing need for the development of mimetic rock surfaces using advanced surface modification techniques. In this work, a novel coating method, called Layer-by-Layer (LBL) self-assembly, is employed to modify the surface of Polydimethylsiloxane (PDMinisymposium) micro-reservoirs [3, 4]. Montmorillonite, a dominant clay mineral in subsurface formations, and Poly (diallyldimethylammonium chloride) (PDDA) are alternatively coated on the PDMinisymposium chips (montmorillonite on the topmost) to mimic homogeneous clay-coated detrital grains. As per coating protocol, the layering is repeated for multiple cycles followed by characterizing the morphology and homogeneity of the clay-coated surface using Scan Electron Microscopy (SEM) and optical microscopy. The SEM and optical images (Fig. 1 and 2, respectively) demonstrated that the PDMinisymposium surface with a proper number of layers was fully (over 99%) covered with microscale clay particles. This demonstration truly represents the natural appearance for most of the subsurface sandstones and all coal and shale rocks. Using contact angle measurements, it was shown that the modified PDMinisymposium surfaces have strong hydrophilic property, mimicking the mudstone surface property, in comparison with the hydrophobic characteristic of bare PDMinisymposium surface. We further examined the coating stability with varieties of oil displacement experiments in microchannels (width: 140 um, depth: 100 um) of surface modified PDMinisymposium microfluidic chips. Cold water, hot water, and surfactant (Tween 80) solutions were injected into the oil-saturated pore network of the modified micro-reservoirs with the flow rate of 0.05 ml/h for 10 times of the microfluidic chip volume respectively. The results revealed that the coatings provide relatively high stability , with only a small amount (less than 5%) of clay particles detach from the surface, flow with the mobile phase, and form patches of original bare PDMinisymposium surface (Fig. 3). Besides, the clay particle swelling was observed upon injection of DI water, building up residual water saturation in flooding experiments. LBL provides a great opportunity to fabricate micro-reservoirs mimicking the real rock pore structure and pore surface properties with potential application for investigation on subsurface flow analysis in mimetic reservoirs.

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MNM3D: a modelling tool for simulation of nanoparticle injection and transport in 3D geometries

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The design of a field-scale injection of engineered nanoparticle (NP) suspensions for the remediation of a polluted site requires the development of quantitative predictive models for the system design and implementation. In general, micro- and nanoparticle transport in porous media is controlled by particle-particle and particle-porous media interactions, which are in turn affected by flow velocity and pore water chemistry. Particle transport is modelled by a modified advection-dispersion equation, which accounts for particle deposition and release phenomena. During the injection, a strong perturbation of the flow field is induced around the well, and the particle transport is mainly controlled by the consequent sharp variation of pore-water velocity, and by the hydro-chemical properties of the injected fluid. Conversely, when the injection is stopped, the particles are transported solely due to the natural flow, and the influence of groundwater geochemistry (ionic strength, IS, in particular) on the particle behaviour becomes predominant. Pore-water velocity and IS are therefore important parameters influencing particle transport in groundwater, and have to be taken into account by the numerical codes used to support nanoremediation design. Several analytical and numerical tools have been developed in recent years to model the transport of colloidal particles in simplified geometry and boundary conditions. For instance, the numerical tool MNMs was developed by the authors of this work to simulate colloidal transport in 1D Cartesian and radial coordinates. Only few simulation tools are instead available for 3D colloid transport, and none of them implements direct correlations accounting for variations of groundwater IS and flow velocity. In this work a new modelling tool, MNM3D (Micro and Nanoparticles transport Model in 3D geometries), is proposed for the simulation of injection and transport of nanoparticle suspensions in generic complex scenarios. MNM3D implements a new formulation to account for the simultaneous dependency of the attachment and detachment kinetic coefficients on groundwater IS and velocity. To the authors' knowledge, MNM3D is the first 3D numerical code embedding a specific routine for the continuous calculation, cell by cell and at the time-step level (for transient flow simulations), of the attachment and detachment kinetics. The software was developed in the framework of the FP7 European research project NanoRem and can be used to predict the NP mobility at different stages of a nanoremediation application, both in the planning and design stage (i.e. support the design of the injection plan), and later to predict the long-term particle mobility after injection (i.e. support the monitoring, final fate of the injected particles). In this work MNM3D is used to model a 2D pilot scale injection of CARBO-IRON® in a small scale flume carried out at the VEGAS facilities in the framework of the NanoRem project. Moreover, the long term fate of an hypothetical release of nanoparticles into the environment from a landfill is simulated.

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Moisture Sorption in Porous Media

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Hygroscopic materials such as leather and fibrous textiles, absorb a considerable amount of moisture when exposed to humid air. Gravimetric experiments were conducted where the materials were maintained at a constant temperature and exposed to humid air (nitrogen, water vapor mixture) in the range of 0-90%. At each humidity level, the materials reached equilibrium with the surroundings. Sorption isotherms obtained in this manner were analyzed using the BET theory. The heat of adsorption as well as the monolayer capacity were determined.

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On immiscible displacement in Slippery Liquid Infused Membranes (SLIM)

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Surfaces with remarkable non-wetting properties can be achieved via the presence of trapping air pockets or pockets with lubricating liquid. The first group of these surfaces, which are inspired by nature (lotus leaf), is known as superhydrophobic surfaces. As long as air pockets are stable in superhydrophobic surfaces, they continue to exhibit non-wetting properties. However, maintaining stable air pockets is challenging. As a result, a new class of bio-inspired interfacial materials, i.e. Slippery Liquid Infused Porous Surfaces (SLIPS), have been introduced recently.[1-2] The principle of liquid infiltration is based on well-matched solid and liquid surface energies, combined with microtextural roughness. The infusion liquid fills the pores and forms a continuous overlying film. The capillary-stabilized liquid in the micro- or nanometer-sized pores leads to a gating mechanism which can coordinate multiphase transport. Some of the remarkable properties of these surfaces such as self-healing, anti-fouling and multi-phase transport without clogging depends on the presence of the liquid-lined pores (adaptive pores) (See Graphic 1).[3-4] In this study, immiscible displacement in SLIMs has been investigated via gas-liquid and liquid-liquid displacement porometry. These experimental studies focus on macroscopic flows in realistic porous materials such as membranes (See Graphic 2). These experiments provide important insight into dynamics of immiscible displacement in the porous network. In order to observe the displacement mechanism microscopically, a microfluidic chip with well-defined surface and geometrical features has been used to study the invasion mechanism in liquid-liquid displacement. Porometry results show the presence of the surface covering liquid film inside the membrane (at the pore surface). Annular two-phase flow models and liquid-liquid displacement porometry theory were used to validate the results. The experimental conditions are kept the same for both porometry and microfluidic experiments by using the same viscosity ratio, capillary number and surface wettability. A highly ramified structure with preferential flow paths (fingers) is observed which is compatible with capillary fingering invasion regime in drainage. Trapping of infusion liquid provides long, fractal interfaces with a patchy pattern.

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Porous microstructure and vapour permeability of traditional canvas paintings

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The characterization of the microstructure of paintings gives better insight in the way they react to changes in ambient conditions. In this paper we study two aspects of the porous system of a traditional oil painting on canvas using different techniques: synchrotron radiation based X-ray micro-CT, conventional X-ray micro-CT, and MIP. The aim is to establish a link between the accessible porosity and the vapour permeability, measured in stationary diffusion tests at different levels of relative humidity (RH) [1]. On one hand we looked at the ground paint layer, a mixture of animal glue and chalk powder. The combination of MIP and synchrotron X-ray micro-CT (Fig. 1) shows that it has 35 % of interconnected pores in size ranges from 2 to 8 micron with pore throats just below the micron. This is close to the lower limit of the size range measurable with this technique. Octopus Analysis software was used to analyse the morphology of the pore system. On the other hand we present a series of tomographic scans of larger specimens, which include the linen canvas. The canvas presents a significant decrease of vapour permeability at high RH, which can be related to the swelling of the fibres, which leads to a decrease in open spaces in between them. Figures 2 and 3 show the same tomographic 2D cross-section at 0 and 95% RH. The presentation includes the discussion on qualitative and quantitative results of the analysis of the 3D images, combined with the MIP and diffusion measurements.

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Preparing multi-pore homogeneous and layered cores for controlled flooding experiments

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Naturally found porous rocks are usually heterogeneous, and this heterogeneity is important when controlled experiments have to be considered for studying multiphase flow phenomena sensitive to homogeneity of the medium. In this study we explore methods to create synthetic nature-like porous media for flow experiments including both micro- and macro-scale heterogeneities. First, a pre-defined sintered glass core was analysed. The pre-defined properties of this core were properties derived from manufacturer specifications for filter discs, a few mm in thickness. The core, however, was several tens of centimetres in thickness and was made out of sintered pure borosilicate glass. Prior to sintering, the glass was crushed, sieved and compacted. The temperature profile of the oven used for sinteringdepended on the grain size being used. Properties of the sintered-glass porous material were evaluated using coreflood experiments and image analysis. We observe that the type of grains do not match the spatial characteristics expected in a natural porous medium; conchoidal fractured grain surfaces. Moreover, even when prepared with the utmost care, the grain frameworks do show heterogeneous characteristics, such as shrinkage fractures, extension of the matrix in circular patterns due to preparation steps, and edge effects along the walls of the enveloping glass tube. In this first phase of our study we realized that a more natural analogue would be essential, i.e. with a known grain-size distribution, with a high sphericity and roundness. Such a selection would ensure a better understanding of the pore framework and corresponding spatial characteristics, like pore volume, pore-throat and pore-neck dimension distribution. We started with various natural materials, where grains and clays are mixed and exist in various proportions. Mineral composition of the rock sample used was quantified using XRD/XRF measurements. We propose a method where the clay phase is the sintering component for quartz grains. Special care is taken to avoid vugs and void spaces due to the passage of gases that are a product of dehydration, dehydroxylation of the clays and oxidation of the organic components. The porous medium has been compared with sintered glass using 3D computer tomography images and subsequent image analysis.

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Quantification of saturation dependent macroscopic dispersion using micro-Positron Emission Tomography

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Understanding the physics of macrodispersion in porous media is important for predicting transport of aqueous CO2 and geochemical reactions in carbon capture and storage projects, quantifying salt water intrusion, groundwater contamination in the vadose zone, and surfactant transport in EOR waterflood projects. The mixing and displacement of one miscible fluid with another in porous media at the continuum scale is controlled by advection and macrodispersion. Macrodispersion includes the process of mechanical dispersion and molecular diffusion. Mechanical dispersion arises from variations in flow path and flow speed due to the tortuous nature of fluid flow in porous media at the pore scale. Molecular diffusion describes the process by which a system with solute concentration gradients is driven to equilibrium which occurs regardless of flow. At high Peclect numbers, such as those describing typical coreflooding conditions, the influence of mechanical dispersion is the dominant source of macrodispersion and influence of diffusion can be neglected. While dispersion is often measured for an entire core or soil column from effluent tracer breakthrough curves, getting in situ measurements of macro-scale dispersion (i.e. sub-core scale) is much more difficult. As a result, there is limited experimental macrodispersion data from real geologic porous media, particularly in multiphase flow conditions. In this study we use micro-Positron Emission Tomography to quantify macrodispersion of tracer pulses injected during single and multiphase flow in a heterogeneous sandstone core. For the quantitative analysis of the PET-derived data, the flow is assumed to be one dimensional along the length of the core at the scale of the voxel dimensions (~2 mm). Within each row of voxels along the axis of the core it is possible to directly calculate macrodispersion using statistical spatial moment analysis at different points in time during the experiments. This results of this study describe the relationship between phase saturation and macrodispersion of tracer as it travels through the core. To our knowledge this is one of the first instances of saturation dependent macrodispersion quantification in real geologic materials and highlights the growing utility of PET imaging for enhancing our understanding of flow at the continuum scale in porous media.

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Real-Time Imaging of Two-Phase Immiscible Fluid Flow Displacement in laboratory scale Porous Media

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We focus on the experimental investigation of the flow of two immiscible fluids (water/oil, or water/gas) in laboratory-scale porous media samples. Rock properties (i.e., porosity and absolute permeability) and two-phase saturation data are obtained on a core sample of a Portland limestone by real-time monitoring of fluid displacement relying on X-Ray CT imaging. Our laboratory scale methodology allows for improved relative permeability characterization through a joint use of traditional flow-through investigations and direct X-Ray measurement with sub-millimetric resolution of the core-wide saturation distribution. The experimental system also imbues us with the capability of documenting the complex dynamics of two-phase displacements according to diverse resolutions, leading to advanced characterization of the effects of local sample inhomogeneity. Our optimized methodology for data-elaboration enables us to obtain one-dimensional (1D) (i.e., section-averaged) information as well as combine a series of two-dimensional (2D) CT slices (raw radiograph) into three-dimensional (3D) views. Results of core-flood experiments document (i) the influence of rock heterogeneities and mobility ratio on volumetric sweep out and (ii) the capability of our experimental methodology to obtain two-phase data for model calibration. It is expected that further development of the technique could provide improved fundamental understanding of key pore-scale processes in porous media, such as hysteresis, snap-off, and non-wetting phase entrapment.

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Separate Effect of Potential Determining Ions and Dilution on Wettability

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Mature oil fields can recover more oil by shifting the wettability to optimum conditions depending on the current wetting state of a reservoir. Flotation experiments were used to differentiate the influence of low salinity (dilution) water from injected or internally produced potential determining anions (PDA's) like sulfate on wettability alteration. We evaluated the separate effect of PDA's and low salinity brines on wettability at different temperatures. The injected or imbibed water that has different ionic strength and composition compared to the formation water (FW) is known as "Advanced Water" and has been employed in two different ways to improve oil recovery. In one approach the ionic strength of the injected water is decreased. While in the other approach ionic composition of the injected water is adjusted [1]. However, most experiments have not isolated these two processes. For instance, substitution of seawater for more saline formation brine lowers salinity but increases sulfate. In the first aspect the concentration of total dissolved solids (TDS) with or without potential determining ions (PDI's) is decreased. In the second aspect of advanced water it is assumed that PDI's adsorb on the rock surface and alter its surface charge. This reversal of surface charge changes the rock-oil polar attraction into repulsion and enhanced the oil recovery. The separate effects of advanced water can be clearly seen in figure (1). In this crude-brine-rock (CBR) system seawater (SW = 36k ppm), seawater without sulfate (SW*0S = 33k ppm) and seawater with borate substituted for sulfate (SW*B*0S = 32k ppm), were tested to change the wettability. The brines were diluted to 20X by adding de-ionized water. The CBR system is oil-wet in full strength solutions whereas water wetting improved in diluted versions. The maximum water-wet conditions were observed at 20X dilution and seawater rich with PDA's shifted the wettability more than the sulfate free seawater. The maximum shift in wettability was observed in borate brine while the minimum in sulfate free seawater. The potential of increasing concentration of sulfate (2.4 mmol to 96 mmol) in seawater at 23, 50 & 100oC was evaluated [1] and the maximum water wetness was observed at 2 mmol/l in this CBR system as shown in figure (2). But on further increasing the concentration of sulfate in seawater the system became more oil-wet and the effect increased up to 96 mmol/l at 100oC. In contrast, the influence of sulfate concentration on wettability at 23 & 50oC is very small. So, it shows that the increasing temperature effect on sulfate adsorption is not linear. Moreover, the CBR system became more oil-wet in seawater as temperature increased to 100oC compared to 23 & 50oC as shown in figure (3).

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Sorption in porous media spatially documented with simultaneous measurements of moisture content and temperature variations

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Vapor sorption in hygroscopic porous media is accompanied by a release/storage of heat. This coupled phenomenon is measured at high spatial and temporal resolution using neutron radiography and high-gage thermocouples. Under isothermal conditions, wood, cellular concrete and plaster undergo a steep relative humidity step change. We see, within 5 minutes, changes in moisture content in the top layer accompanied by a rise of temperature. Indirect determination of the heat indicated that the source of heat is the heat of vaporization rather than the heat of sorption. Experiments in which moisture content and temperature variations during the sorption (desorption) process are acquired simultaneously at high temporal and spatial resolutions were conducted. Specimens of cellular concrete, wood (along the three grain orientations) and plaster, 85 x 35 x 10 mm3, are placed in a micro wind tunnel, with their top face exposed to controlled air flow. Dry samples undergo a 0 to 90% RH and moist samples (conditioned at 90%RH) a 90 to 0% RH step change, for 90 to 120 minutes. The air temperature is maintained constant at 23°C. Throughout each experiment, the moisture content variations are imaged with cold neutron radiography at the ICON beamline of the Paul Scherrer Institute (Villigen, Suisse), and thermocouples inside the specimen monitor the temperature variations. The tunnel is mounted on a high-precision balance to obtain the total mass variation during the whole experiment. Experiments were performed for two wind speeds, 0.3 m/s or 1.5 m/s. Total sorption/desorption is compared. Wood in longitudinal orientation has the largest total moisture content variation, up to 4% MC, while plaster has the smallest, less than 0.3% MC. The cold neutron radiography images allow to determine quantitatively the moisture content fields within the media. We note that, although the total uptake is similar for wood (tangential orientation) and cellular concrete, the distribution is different: the moisture front penetrates relatively uniformly in cellular concrete, while only the top 5 mm are active for wood (tangential orientation). Wood orientation has a significant influence on the total variation and the moisture distribution pattern. The co-occurring temperature measurements acquired during sorption and desorption show significant temperature variations within the samples. The largest, in the order of 7°C, is seen in wood (longitudinal orientation). . The temperature variations are about 4°C for cellular concrete and 2°C for plaster. These temperature variations are spatially and temporally linked to the local moisture content variations. The results are analyzed in terms of released/stored energy and can be presented in 2-D, as images at different times. The measured heat effect includes the heat of sorption and the latent heat. For each material, the potential total energy variation is calculated and compared to the energy variation related to the measured temperature variations. The performance of the three materials is compared and discussed in terms of their porosity, hygroscopicity and specific heat. The energy variation related to the measured temperature variations is higher than the

heat of sorption alone, but significantly lower than the heat of vaporization for the adsorbed amount of water, indicating that there is a heat of sorption effect at very low moisture contents (less than 2% for wood, for example), but that the observed temperature variations are mostly due to the heat of vaporization. The use of sorption (desorption) as an energy management tool is worthy of consideration, as it may help reduce energy consumption. The combined temperature/moisture content data in high temporal and spatial definition are unique and are used to further the understanding of the heat effects of sorption and to optimize systems operating at very low moisture content.

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Tank Experiments and numerical Modeling of Macrodispersion of Density-dependent Transport in stochastically heterogeneous porous Media

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Experimental and numerical investigations of density-dependent flow and solute transport in a sand-packed laboratory tank are important for the understanding of such processes in real aquifers. At the hydraulic laboratory of the University of Kassel such experiments are performed in a Plexiglas tank with dimensions 9.8 x 0.1 x 1.225 m, with the main objective to analyze macro-dispersive effects on a fresh-saltwater interface within the heterogeneously-packed sand structure with given stochastic properties. Previous experiments have been carried out with three representative realizations of stochastic heterogeneity with predefined variances Sigma^2 ranging from 0.25 - 1.5 and correlation lengths Lambda_x, Lambda_z of 0.2 - 0.4 m and 0.05 - 0.2, respectively, of the Y=Ln(k) logarithmic permeability field. These experiments investigated the hydrodynamically stable case of a layer of saltwater of different concentrations injected underneath a layer of de-ionized and degassed water. In each stochastic realization, the anisotropic sand structures have been packed in the form of 2401 discrete sand-blocks of dimensions 0.2 X 0.025 m with eight different pre-sieved classes of chemically pure industrial quartz-sands. The hydraulic conductivities of the sands ranged from K = 10^-2 to 10^-4 m/s, corresponding to a permeability range of k = 10^-9 to 10^-11 m^2. Numerous experiments with saltwater (chemically pure NaCl-solutions) concentrations ranging from C_0 = 250 (fresh water) to 100000 ppm (brine) and flow velocities ranging from v = 1 to 8 m/d were carried out in each sand pack realization. Depending on the prescribed flow velocities, steady-state conditions for the solute transport, i.e. of the mixing zone across the fresh-saltwater interface, were obtained after a duration of one to three weeks. In this contribution we report on the results of new sets of tank experiments with an extremely stochastically heterogeneous sand-pack realization. This has been feasible by employing new sand classes covering a wider range of the hydraulic conductivity K. More specifically, 10 sands with K in the range of 1.1*10^-1 to 1.3*10^-4 m/s allow for random packing distributions across the tank, following stochastic turning bands method (TBM) realizations with Y = ln (K_mean) = -5.6, and variance Sigma^2 = 3.06, and correlation lengths of Lambda_x = 0.75 m and Lambda_z = 0.1 m. One of these stochastic realizations was used as a prescription for the tank packing, as described above. For calibration and validation purposes, the experiments are accompanied by numerical simulations using the flow and transport model SUTRA. Together with additional tank experiments of this new stochastic porous-medium representation, the present analysis complements earlier work of Koch and Starke (2001, 2002, 2003, 2006) with regard to this scientific topic, namely, an exhaustive characterization of density-dependent and transversal macro-dispersion in stochastically heterogeneous porous media.

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The Influence of Convection and Diffusion in Fracture During CO2 Injection Progress for Tight Oil EOR

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Due to the high conductivity of rock fractures, convection and diffusion in fractures affect the efficiency of mass transfer between fracture and matrix significantly during gas injection process. It has been a main oil recovery mechanism, especially in tight reservoirs with extremely low-permeability rock matrix. In current studies, many authors usually illustrate this process based on inconsistent models and reduce the fracture to a lower-dimensional structure to simplify the simulation process. In this paper, we developed a coupled model to demonstrate the effect of convection and diffusion in fractures on the composition of fluids in the porous rock matrix without those simplifications. The improved model accounts for convection and two dimensional diffusions in the fracture. Vertical convection and diffusion in the matrix is considered as well. We also incorporated the interaction between matrix and fracture by exposing a consistent boundary condition at the fracture wall. Subsequently, a numerical method was applied to solve the model and the distribution of injected gas concentration in both fracture and matrix. The results were compared with our available experimental data for validation. Finally, we combined the proposed model and the compositional model together to calculate the composition of each component as well as saturation in the matrix at each time-step during CO2 injection process. The results show that the existence of convection and diffusion in fracture enhanced CO2 transport in the porous matrix. And convection in fracture favored transversal vertical diffusion both in fracture and matrix, which is the main mechanism for fracture matrix mass transfer. With decreasing matrix permeability, transverse vertical diffusion in matrix dominated in mass transfer gradually. As a result, both transport mechanisms of injection in the fracture will cause an appreciable impact on the composition of fluids in the matrix. It implied that this process could lead to a significant improvement of final recovery. The proposed model shed some light on mechanism of mass transfer in gas injection for tight oil reservoirs. The method provided EOR practice for reference.

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What we can learn about transport, dispersion and adsorption of colloidal particles from MRI (Magnetic Resonance Imaging)

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The use of nanoparticles, which can give interesting properties to many products, has considerably grown in the last 50 years. However, their release in the environment can cause dramatic pollutions and is difficult to evaluate. As a consequence, it is important to be able to predict precisely their transport and retention in porous media such as soils. In order to explore the possibilities of MRI to get such information we studied transport, dispersion and adsorption in various porous media (glass beads, sand and soil agregates). We first look at particle transport through homogeneous bead or sand packings at different flow rates from MRI visualizations of transport characteristics of a pulse of (negatively charged) paramagnetic nanoparticles. Through 2D imaging we observe that particles are transported through the pores at the same average velocity all along the sample. We also observe homogeneous dispersion inside the sample, but it appears that entrance effects may induce significant radial heterogeneities, which would affect the interpretation of breakthrough curve. Another MRI approach (i.e. 1D profiles along sample axis) provides quantitative measurements of the evolution in time of the longitudinal particle distribution in the sample [1]. These data can be analyzed to deduce the coefficient of dispersion independently of entrance effects. The values obtained for this “effective” dispersion coefficient in the range 100-10000 of Peclet numbers are almost ten times lower than the commonly admitted values (see graph 1). Then we focus on the combined effect of transport and adsorption by injecting positively charged particles in two types of porous media (sand and model soil aggregates). In order to get quantitative information we carry out 2D and 1D measurements of the evolution in time of the distribution profile of all particles (suspended or adsorbed) in cross-sectional layers along the sample axis during the flow. We show that the analysis of the results of injection of successive pulses of a particle suspension make it possible to get a clear description of the adsorption process. [2] For the sand columns it appears that particles rapidly explore the pores and adsorb as soon as they encounter available sites on grains, and the surplus of particles go on advancing in the sample. In that case further analysis of the profiles makes it possible to distinguish the respective concentration distribution of suspended and adsorbed particles over time at each step of the process. For the model soil columns, adsorbed particles are not detected but it is possible to analyze the successive profiles of suspended particles to extract the distribution of adsorbed particles in time. In that case we deduce that the adsorbed fraction results from a partial exploration of aggregate surface, a process which may be described with a simple physical model.

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1D analytical solution of polymer slug injection with viscous fingering

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Water injection is the most common method to simultaneously displace oil and maintain reservoir pressure. Polymer can be used to increase the viscosity of water and in turn reduces its mobility relative to the oil. A more stable and relatively slower aqueous front displacing oil is obtained, thus improving the overall macroscopic displacement efficiency. This strategy is particularly relevant in today's era where more favourable fields with light crude have been exploited and produced.

Similar to other techniques of enhanced oil recovery (EOR), the financial cost of polymer injection is very high. The main contributing cost is the polymer itself, incurred continuously as operating expenditure (OPEX). A more optimum operation can be achieved by having a polymer slug instead of continuous injection. In this case, after polymer has been injected for a certain period, chase water (which contains no polymer) is introduced. There is, however, an issue with this strategy. As chase water is less viscous and more mobile, viscous instability in the form of fingering may occur and possibly destroy the polymer slug and reduce the overall recovery efficiency.

The continuous polymer injection in 1D model can be solved by considering oil-polymer and oil-water fractional flow curves (Pope, 1980). The main feature of this type of displacement is the existence of an additional shock front due to the formation of connate water bank, which can be found by performing a "jump" between the two fractional flow curves. Analogous to Buckley-Leverett analysis, the water saturation profile can be calculated by using the method of characteristics. The self-similar variable x/t is used to reduce the partial differential equation describing the transport of water using fractional flow formulation to an ordinary differential equation.

The analytical solution for polymer slug is less trivial. The discontinuity caused by the introduction of chase water into the system means x/t variable can no longer be used to solve the problem. Bedrikovetsky (1993) showed how the chase water front can be tracked by conserving the polymer slug volume injected using Green's theory for closed curve. However, the effect of viscous instability caused by less viscous chase water was not considered here, making it less applicable to more realistic problems.

The main objective of this paper is to propose an analytical solution in 1D model to predict the breakdown of the polymer slug in secondary oil recovery. We first derive the position of chase water front as a function of time using simple integration, assuming no fingers are being formed. This gives similar results as those previously presented by Bedrikovetsky. These are then extended to capture the viscous instability effect, by assuming that the average mixing effect of fingering can be represented by the empirical Todd-Longstaff model (1972). This allows us to ultimately predict when a polymer slug will break down. These results are then compared against numerical solution as well as high resolution first contact miscible simulation. The analytical solution presented here can be used to rapidly determine the optimal polymer slug size, which is potentially very useful during EOR screening studies.

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Anomalous behavior of hysteresis of fluid displacement in mixed wet granular piles

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We investigate experimentally the impact of heterogeneity on the capillary pressure hysteresis in fluid invasion of model porous media. While enhanced heterogeneity is usually known to increase hysteresis phenomena, we find that hysteresis is greatly reduced when heterogeneities in wettability are introduced. On the contrary, geometric heterogeneity (like bi-disperse particle size) does not lead to such effect. We provide a qualitative explanation of this surprising result, resting on rather general geometric arguments.

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Applications of multiple-point statistics in the reconstruction of heterogeneous porous networks in continental carbonates

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Multiple-point geostatistics is a statistical method that has been successfully applied in the modelling of reservoirs. In contrast to classical variogram based simulations, spatial connection and reservoir complexity is preserved (Guardiano & Srivastava, 1993; Mariethoz et al., 2010). Multiple-point statistics take a training image and conditioning data as input. The patterns of the former are fitted to the latter by a pixel-wise reconstruction. The approach of multiple-point statistics could be applied in the modelling of pore networks of continental carbonates. These rocks contain the most complex natural pore networks and have pore sizes between nanometer and meter scale. From a large dataset of these carbonates, it turns out that no distinct correlation can be made between porosity and permeability (Soete et al., 2016). To determine what causes scatter of data, connectivity should be visualized. At present, this is done with computed tomography (CT) where microfocus CT provides small scale details and medical CT only visualizes large pores because of inherent resolution ranges of both systems. For optimal visualization of connectivity and realistic modelling of permeability, both scales should be combined in multiscale models. Such models could be generated through multiple-point statistics when high-resolution data is used as training image and low-resolution as conditioning data (Claes, 2015). Prior to such simulation a pre-processing step is applied to separate large and small pores in the high resolution training image. Only small pores will be simulated from the training image, while preserving connection to large pores. This step reduces the overestimation of porosity from 130% to 30% in a conceptual binary pore system (Figure 1). To obtain as much information as possible in realistic samples, it is proposed to use multiple training images, that are stored in a digital rock library. Such a library provides a collection of digital models of porous networks, separated by rock lithotypes, a classification based on texture and porosity. The benefit and need of such a classification is demonstrated on a 2D image, in which three different lithotypes are recognized. Simulations on this example show a reduction of mismatch with the original image from 5.9% to 2.8%, simply by differentiating lithotypes (Figure 2). Multiple-point statistics have another application that could extend the multiscale approach. This application models a 3D volume from 2D data and a rock library. In geological studies, 2D data is usually obtained by classical microscopy, scanning electron microscopy (SEM) and field pictures. In previous studies by Okabe and Blunt (2005) and Claes (2015), two approaches are proposed to go from a 2D section as training image to 3D volume. Both are assuming homogeneity of the system and are based on sequential 2D simulations. The methods are tested for heterogeneous pore models and although there is visual resemblance to the original pore structure, the porosity is overestimated by factor 2 and connectivity is forced. Future simulations will expand the Okabe and Blunt (2005) workflow to three training images to have heterogeneity better represented and statistical data of the digital rock library could be included in the models (Figure 3).

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Architecture of ordered mesoporous carbon spheres@Tin dioxide core satellite nanostructures for enhanced high-rate lithium storage

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A novel highly ordered mesoporous carbon nanospheres (OMCS) embedded with ultrafine Tin dioxide nanoparticles was successfully fabricated and used as a promising anode material for excellent rate capability and durability of Li ion batteries (LIBs). The uniform OMCS with mean size of 90 nm was fabricated as core materials and then embedded with 3-6 nm Tin dioxide as satellites at various Sn/C weight ratios of 15-35% to form the OMCS@Tin dioxide nanocomposites by microwave-assisted hydrothermal method. The core-satellite nanocomposites with interconnected micro-meso-macroporous channels not only shorten the diffusion pathway of ions and electrons but can also enhance the electrolyte accessibility for rapid ions transport at high rate. Remarkably, the OMCS@Tin dioxide at Sn/C ratio of 35% exhibits an excellent reversible capacity of 1770 mA h g-1 at 35 mA g-1 initially and then maintains at 400 mA h g-1 under an ultra-high current density of 3500 mA g-1 after 400 cycles. The OMCS cores provide excellent conductive and mechanical stabilities for rapid lithiation reaction, while the intimate contact of Tin dioxide nanocrystals with OMCS shortens the electrons transfer paths and constrains the volume expansion during lithiation/delithiation, resulting in the enhancement of stable lithium storage capacity at high current density. In addition, the formation of zerovalent Sn nanoparticles with stable SEI layers after the first cycle enables the carriers to transfer electrons more readily. Results obtained in this study clearly demonstrate the superior electrochemical performances of OMCS@Tin dioxide core-satellites nanostructures and can open an avenue to fabricate novel carbon-metal oxide nanocomposites as anode materials for high-rate LIBs.

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Automatic estimation of contact angle from pore-scale X-ray 3D-images

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A new approach is presented to measure the in-situ contact angle (θ) between immiscible fluids, applied to pore-scale X-ray images. To validate the approach, we first study wide range of contact angles of a spherical droplet of oil residing on a flat solid surface surrounded by brine, using synthetic 3D images of different resolutions (1/10th, 1/14th, 1/28th and 1/56th). We then apply this method to experimental data of oil/brine fluids at the pore-scale used from (Singh K. et al, 2016), which imaged at reservoir conditions (10MPa and 50 celsius) inside a quarry limestone using X-ray microtomography.

In this method, we define vectors that have a direction perpendicular to a surface. The contact angle is found from the vector dot product of vectors describing the oil/brine interface and the solid surface, where they meet at the three-phase contact line. We are able, automatically, to generate contact angle values representing each invaded pore-element in the image.

The final measured results for the synthetic images show high accuracy, with less than 1% difference between the average measured and the ideal contact angle, for all used resolutions. Also, for the used experimental data, the algorithm results show almost perfect match with the final mean contact angle, and more narrowed dirstribution with less mean deviation. Furthermore, the potential of this automatic approach in measuring contact angles at the pore-scale is presented and discussed.

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Calculating geometric tortuosity by the use of the Path Tracking Method

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Path Tracking Method is an iterative method of determination of the length of a pore channel in a granular porous medium in the chosen space direction, which consists of analysing the local structure of the pore space based on the information about the location and diameter of every particle forming the bed. The PTM method was developed by the author in 2009, as a tool destined for investigating the spatial structure of granular beds [1]. As a result, the numerical code called PathFinder was written [2], currently freely available in the Internet. The length of a pore channel in the PTM is determined between two parallel planes, based on the sum of the unitary lengths. This method is based on the so-called tetrahedral structures that establish the basis for the calculation algorithm. Tetrahedral structures are created based on the data on the location and diameter of each particle in the bed. Such data may be obtained from the use of the Discrete Element Method or from the analysis of a set of tomography scans [3]. An interesting possibility of the use of the PTM method is the so-called Regular Grid Method (RGM), which allows obtaining thousands values of the paths lengths for one porous bed in a very short time [4]. In a consequence, performing a statistical analysis is possible or other investigations related to the geometric tortuosity.

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Conceptual Theories to Develop Naturally Fractured Reservoirs

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Until now in order to produce oil from naturally fractured reservoirs, some vertical wells are drilled. During production, due to pressure reduction, Gas Oil Contact level moves toward production wells and in other word gas invaded zone expands. The main problem of fractured reservoirs is oil trapping in matrices of gas invaded zone. when gas invaded zone expands high enough, vertical wells should be transformed to horizontal ones. Which means that the vertical production wells should be shut and drilled in horizontal direction and oil production will continue until reservoir pressure decreases lower than bubble point pressure. Since naturally fractured reservoirs are formed from matrices and fractures, there are many restrictions to manipulate enhanced oil recovery methods. The most important restriction is fluid flooding. When a fluid is injected to the fractured reservoir, it moves toward production wells through fractures due to high pressure gradient and sweeps oil exists in fractures and not matrices. In this paper in order to increase recovery of naturally fractured reservoirs from the beginning of production until abandonment of the reservoir, three conceptual methods will be suggested.

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DGFlow: modelling backward erosion piping using a finite element code

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In the Netherlands, backward erosion piping (BEP) is considered to pose a significant threat to the stability of dikes and levees that are founded on sandy or silty strata (van Beek et al., 2015). During a period of high-water level in the river, seepage forces transport sand grains along the interface between the cohesive dike body and the sandy substratum, leading to the formation of small pipes. Given that the water level is high enough for a sufficiently long time, these pipes can propagate upstream, which leads to progressive erosion, widening and deepening of the pipes, and the eventual collapse of the overlying structure. Currently the Sellmeijer rule is used to assess the risk of BEP in the Netherlands; this rule predicts the critical head difference, defined as the difference in river water level and polder water level, that a dike can withstand. The Sellmeijer rule is based on the Sellmeijer model, which accounts for the force equilibrium on the grains in the pipe and the groundwater head distribution in the aquifer (Sellmeijer, 1988; Sellmeijer et al., 2011). The pipe is considered as a channel with infinite width, and particle erosion is based on White's limit state equilibrium and viscous flow equations. The Sellmeijer model for the limit equilibrium in the pipe has been implemented as a boundary condition in the groundwater flow program Minisymposium eep, which can be used to determine the critical head for stationary flow situations (Sellmeijer, 2006). D-Geo Flow is a new finite element groundwater flow code in which the limit equilibrium in the pipe has also been implemented (Van Esch et al., 2013). The groundwater pressure field is solved based on the Richard's Equation, allowing transient flow calculations, which are not possible in Minisymposium eep. This contribution discusses the implementation of the equilibrium condition in D-Geo Flow and compares this to the implementation in Minisymposium eep. Cases with a uniform and a stratified subsurface are computed in both models and compared to the critical head that is obtained by using the calculation rule. Validation of the results from the two models focuses on the accuracy with which the limit equilibrium is fulfilled, the dimension of the pipe and the resulting critical head. These show that the implementation of the limit equilibrium, and numerical discretisation have a significant effect on the accuracy with which the limit equilibrium is computed in Minisymposium eep and D-Geo Flow. This results in a small but consistent difference between the critical head computed with the two models. Comparison of the results for homogeneous and stratified aquifers to the Sellmeijer calculation rule show that this rule can significantly over- or underestimate the critical head for stratified situations . By providing a means to more accurately account for the subsurface stratigraphy, and time dependent boundary conditions D-Geo Flow allows for a more realistic assessment of the risk of piping than the Sellmeijer calculation rule and Minisymposium eep.

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Dielectric properties of Natural porous media

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Fontainebleau sandstone is a unique uncomplicated natural porous medium (Zinszner, 2007). It mostly consists of pure Quartz (0.995 wt%) and an almost constant grain size, despite its considerable porosity change (generally 0.02 to 0.3) (Thiry et al., 1988). It provides us with the ideal spatial properties to investigate the elementary dielectric behaviour in natural porous media.

Figure 1: Fontainebleau Sandstone. Left: SEM Image , Right: Thin section

To evaluate the Dielectric properties, the following steps are taken: 1- We visualize and quantify spatial attributions of the grain and pore matrix by CTs, SEM, thin section (Figure 1) image analysis, associated to stereological measurements and statistical 2D/3D reconstructions. This is to understand the heterogeneity of the quantified grain- and associated pore-framework and the possible impact of clay.

2- We measure the conductivities of the porous media following the method of conductivity of fully saturated cores with different brine concentrations (Figure 2). It provides, among others, the Formation factor and cementation exponent.

3- We measure the surface charges (i.e. electro-kinetic forces) of the grains for one material, using two different approaches (Zeta sizer) and streaming potential coefficients.

Figure 2: Saturated Sandstone brine conductivity versus porosity.

Porous medium of Fontainebleau sandstone has a homogeneous texture. Follows the first Archie relation for clean sandstones, it is proven that clay minerals are accessory or almost non-existent and it does not have an impact on the electrical conductivities. The cementation exponents show that the quartz overgrowth is evident and causes reduction of the permeability by reduction of pore throat area and coordination number. The surface charges of Fontainebleau's grain are negative due to the presence of the quartz.

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Displacement diffusion in a gravel column-reinforced soil based on a probabilistic approach

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Harr (1977) proposed an approach in which diffusion of stresses in a granular medium is based on probability theory. The approach is revisited using the diffusion of vertical displacements in the granular medium to account for a gravel column-reinforced soil submitted to foundation loading (Bourdeau, 1986). An applied point load on the surface of a granular media will follow an erratic path, depending on the probability of transition between the grains. The diffusion of the expected vertical stress in the granular medium obeys a similar equation as the known Fokker-Planck equation. The parameter of diffusion is shown to approximate the mean diameter of the grains of the material. A numerical approach based on finite elements method is used to account for a gravel column-reinforced soil submitted to loadings of a building foundation. The obtained results show that the diffusion of displacements in the granular medium is influenced by the grain size distribution and it helps using the method as a valuable tool to calculate settlements. Comparisons are shown when the soil (granular medium) is reinforced with gravel columns.

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Dynamic time warping applied on NMR depth profiles

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Since the invention of the NMR-MOUSE® in 1996 [1] and its more advanced derivate called the Profile NMR-MOUSE, unilateral NMR devices have shown to produce in-situ depth profiles with a resolution down to 2.3 µm [2]. The maximum penetration depth of these devices depends on the size of the sensor and reaches up to 25 mm. The NMR-MOUSE® is applied to visualize sub-surface effects and to reveal potential layer structures. In suitable samples, depth profiles can be utilized to visualize stratigraphy. However, two problems arise when comparing stratigraphy from large numbers of samples. For one, the sheer number may be too high to visualize the differences and similarities of all profiles by manual comparison. This problem has since been solved by applying a method of statistics called principle component analysis (PCA) [3], thereby projecting all data sets onto one plane, which is constructed by two principle component axes. Similarity between datasets is observed when the distance between points is low. However, PCA is a black-box method where the axes are ill-defined parameters only determined by the complex statistical analysis. The second problem that occurs and sometimes impedes the use of PCA is that the layer structure in a sample may be very similar while sometimes the individual layer thicknesses may differ. We present a method of correlating any depth profile with any other reference data set using a process known as dynamic time warping. The algorithm is more commonly used in speech recognition software and can stretch the x-axis nonlinearly when comparing two one-dimensional datasets, thereby eliminating potential differences in layer thickness. Consequently, mismatch of profiles arises only due to different stratigraphy. Depth profiles of moisture in Roman wall paintings and frescos from Herculaneum were treated with dynamic time warping due to their large number acquired over multiple visits to the site in the last 5 years. By selecting a few representative profiles as references it was possible to quantify their similarities and differences along a simple correlation matrix. This process automatizes the separation of profiles in regard to the references which correspond to styles of wall making.

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Effect of Freeze - Thaw Cycle on the Weathering of Arkose Containing Concretions

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The statues of Yungang grottoes of China, which has important artistic and historical value, were engraved on arkose. There are many pores in the arkose. Moreover, feldspar minerals can be dissolved to some extents in acidic aqueous media, leading to the formation of secondary pores. Water can flow slowly through the arkose by seepage, which leads to various types of weathering. The minimum and maximum temperature of Yungang grottoes is about -30℃ and 30℃, respectively. During the past thousand years, Yungang grottoes has suffered a lot from the f freeze-thaw cycles. There are many concretions in arkose. The region near the interface is heterogeneous. Freeze-thaw cycle can cause significant weathering of arkose containing water, especially in the interface between arkose matrix and concretions. In order to research the weathering phenomenon of arkose containing concretions, the fissure's propagation rule of arkose selected from Yungang grottoes during different freeze-thaw cycles is studied by using laser confocal microscopy, XRD, SEM and EDX to observe crack initiation, extension, and elongation process in three typical regions. The results show: (1) fissures generate in the interface between concretions and arkose matrix firstly, after 5 cycles of freeze-thaw; (2) the width of fissure increases with the cycles of freeze-thaw, and the fissures extend along the interface; (3) the center of concretions generate a single fissure after 10 cycles of freeze-thaw; (4) with the increase of the number of freeze-thaw cycle, the concretions centre continues to generate new fissures and the early fissure extends and elongates, forming fissure network; (5) the fissures exist in the arkose matrix after 20 cycles of freeze-thaw, and that expand slowly. Fissures develop generally in regions with high heterogeneity. The concretions significantly enhanced the heterogeneity of arkose. Heterogeneity is the internal cause that the arkose of Yungang grottoes generates cavernous weathering.

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Effect of water salinity on rock resistivity during waterflooding

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As a secondary oil recovery method, waterflooding is wildly used in long-term production oilfields. When the injected water salinity is similar with original formation water, remaining oil can be easily calculated by resistivity logging. However, different oilfields use water in various salinities, leading to oil saturation calculation difficulties. In order to investigate the effect of water salinity on rock resistivity quantitatively, we used digital rock techniques. We first constructed 3D digital rock model based on process-based method, and then we used finite element method to calculate rock resistivity. Determining accurate input parameters are vital for resistivity calculation, such as original water resistivity and free water resistivity in whole 3D pore space. Different degrees of water injections may cause huge water resistivity differences. We assumed the water-injection process contained three stages: non-water-flooded stage, low and medium water-flooded stages, and high water-flooded stage. For characterising mixed water resistivity, we divided bound water into two parts: surface bound water in big pores and bound water in small pores. The injected water first contact the surface bound water in big pores and then contact the bound water in small pores. Through combining and modifying parallel resistivity model and ion exchange-based resistivity model, we developed a novel method to calculate mixed water resistivity. Finally we changed injected water salinity in digital rock models to study rock electrical properties. The results show that there are specific phenomena between water saturation and rock resistivity. When the salinity of injected water is low (fresh-water), the relationship between water saturations and rock resistivities formed S- shape curve. However, when the salinity of injected water is high (salt-water), rock resistivity would be decreased with the increase of water saturation. The trend of calculated resistivity curve agree with experimental result, which also verifies our numerical simulation method.

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European Project NANO-CATHEDRAL Efficacy assessment of nanomaterials for conservation of natural stones: the impact of pore structure in selecting appropriate conservative treatments

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The project NANO-CATHEDRAL [1] aims at developing new materials, technologies and procedures for the conservation of deteriorated stones in monumental buildings and cathedrals and high value contemporary architecture, with a particular emphasis on the preservation of the originality of materials and on the development of a tailor-made approach to tackle the specific problems related to the different lithotypes. In fact, the objective is providing “key tools” in terms of innovative nano-structured conservation materials, for restoration and conservation on a full European scale, thanks to the research work made onto lithotypes representative of different European geographical areas and styles and of different climate and environmental conditions. Five different cathedrals were selected as they may be considered as representative of both different exposure conditions and different types of stones. In particular, the Cathedral of Pisa, in central Italy, and the Cathedral de Santa María of Vitoria-Gasteiz in Spain were selected as representative of south European “Mediterranean” climate in coastal and continental regions, respectively; the Sint-Baafs Cathedral of Ghent, in Belgium, the Cathedral of St. Peter and Mary in Cologne, Germany and the St. Stephen's Cathedral, in Wien, Austria, were selected as representative of North European climate in coastal and continental regions, respectively. Moreover, the Oslo Opera House, was considered as an example of a contemporary building coated with white Carrara marble. The selected stones represent different lithotypes, such as marble, sandstone, limestone, characterised by a ranging of petrographic and porosity features. A general protocol has been defined for the identification of the petrographic, mineralogical, textural and structural features of the stone materials, the identification of the degradation patterns, the evaluation of the causes and mechanisms of alteration and degradation also in function of pore structure of stones [2]. A selection of nano-structured innovative formulated products, such as nano-particle based consolidants, and proper polymer nano-composites based coatings are currently testing onto stones. Efficacy of selected products by proper measurements is under study by applying a multidisciplinary protocol, to verify their consolidation and protection action; as regard consolidants, investigations are especially focused on evaluating the ability of products to penetrate the inner structure of selected stones, a feature that greatly depends on the characteristics of the product itself but also on the porosity of the substrate material. Dedicated modelling, tailored characterizations, standardization of the production and treatments application will be the next step activities of the NANO-CATHEDRAL project, aimed at enabling decision makers the access to restoration and conservation with a systematic awareness based on in situ systematic experimentations.

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High strength self-supporting geopolymer and zeolite sieves for cesium removal

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This paper summarizes a portion of the experimental work recently conducted by the authors [1]. Geopolymers and zeolite are often considered analogous of each other despite the fact that geopolymers are amorphous to semi-crystalline and zeolites are crystalline [2]. Geopolymers, having high strength and durability, mostly regarded as green cements, while pulverized zeolites have wide industrial applications such as catalysts, gas separators, and ion exchangers [1]. It is a proven technology that the amorphous geopolymeric gels can be hydrothermally converted to crystalline zeolites, increasing the surface area and porosity of dense geopolymeric gels [3,4]. Owing to the structural differences of geopolymer and zeolites, the hybrid geopolymer-zeolite materials can provide a way to synthesize high strength self-supported sieves [1,4]. In this study, mesoporous geopolymers containing nano-crystalline zeolites were synthesized following the procedure reported in our previous study [4]. Industrial by-products such as coal fly ash and granulated blast furnace slag (BFS) were used for synthesis of high strength self-supporting geopolymer and zeolite sieves (may also referred to as bulk-type adsorbents) [1,4]. After hydrothermal treatment, batch adsorption experiments were conducted on cesium radionuclide [1]. In addition, reaction kinetics were studied by employing different contact times of adsorbate with adsorbent [1]. Removal efficiency and capacity of the bulk-type adsorbents were found to be 96% and 15.24 mg/g, respectively. The details of experiments and discussions will be presented.

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Mathematical modeling of optimal membrane filtration

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Membrane filters - essentially, thin sheets of porous medium which act to remove certain particles suspended in a fluid that passes through the medium - are in widespread industrial use, and represent a multi-billion dollar industry worldwide. Major multinational companies such as W.L. Gore & Associates, and Pall Corporation, manufacture a huge range of membrane-based filtration products, and maintain a keen interest in improving and optimizing their filters. Membrane filtration is used in diverse applications, including water purification; treatment of radioactive sludge; various purification processes in the biotech industry; the cleaning of air or other gases; and beer clarification. While the underlying applications and the details of the filtration may vary dramatically (gas vs liquid filtration; small vs large particle removal; slow vs fast throughput; rigid vs deformable particles), the broad engineering challenge of efficient filtration is the same: to achieve finely-controlled separation at low power consumption.

The desired separation control is to remove only those particles in a certain size range from the input flow (often referred to as "feed''); and the obvious resolution to the engineering challenge would appear to be: use the largest pore size and void fraction consistent with the separation requirement. However, these membrane characteristics (and hence the filter's behavior and performance) are far from constant over its lifetime: the particles removed from the feed are deposited within and on the membrane filter, fouling it and degrading the performance over time. The processes by which this fouling occurs are complex, and depend strongly on several factors, including: the internal structure of the membrane; the flow dynamics of the feed solution; and the type of particles in the feed (the shape, size, and chemistry affects how they are removed by the membrane).

Though the fouling literature is extensive, a complete and coherent predictive framework that can realistically describe all fouling modes of a membrane filter is still lacking. A recent review by Iritani [1] concludes by noting that "...further development of simple yet effective mathematical models for elucidating the complicated pore-blocking phenomena in membrane filtration would be highly desirable for guiding decisions on the optimal choice of the membrane and membrane-cleaning strategy in industrial use.''

In this talk we will describe some of our recent and ongoing work on first-principles modeling of membrane filtration and fouling [2,3]. Particular emphasis is paid to how membrane filter design (in particular, permeability gradients across the membrane, and the internal branching structure of pores) can significantly affect filtration efficiency, as measured by (i) total throughput over a filter lifetime, and (ii) proportion of particles removed from the feed.

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Modeling filtration through pleated membrane filters

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Pleated membrane filters are used in a variety of applications due to many advantages that they have over unpleated ones. Understanding the flow and filtration in a complicated geometry associated with pleated filters is however not a simple task. This talk focuses on the first principles modeling of such a problem, describing the flow through porous material surrounding the membrane, and the membrane itself. The model itself builds upon recently published work [1], that presented a tractable and realistic mathematical model describing flow in a pleated filter geometry. That work focused on the membrane fouling by two mechanisms: adsorption of small particles within the pores, and blocking of pores by large particles. In the present talk, this model will be supplemented by consistent and careful modeling of the flow not only in the membrane, but also in the surrounding porous layers. Coupling of the flow in the different domains through suitable realistic boundary conditions allows for formulating a reasonably simple model that is still able to describe accurately the filtering process, without requiring large scale simulations.

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Modelling of pore formation in porous polymer membranes during phase inversion process

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Direct modelling of different preparation processes of polymer membranes is highly challenging. The basic mechanism to prepare polymer membranes is based on precipitation of a polymer solution which then separates into two stable phases forming pores and matrix of the membrane. Since the underlying physical processes (e.g. phase decomposition, coarsening, gelation, etc.) are observed on different time and length scales, the computational effort is immense for molecular simulations. In addition, the detailed mechanisms are not totally understood in theory and most of the explanations came from experimental observations. Therefore, it is recommended to find a fundamental theory to explain all observed effects on morphology of polymer membranes. In the last years it became more visible for Engineers to use Non-equilibrium thermodynamics [1],[2]. This enables us to develop predictive models for the pore formation mechanism of porous polymer membranes based on the measurable quantities like diffusion coefficient or viscosity. In this talk we present a model to dynamically simulate pore formation of porous polymer membranes during phase inversion process. The model enables us to express the final membrane morphology in terms of a thermodynamic and a kinetic parameter. We discuss the influence of a so-called pore builder on the morphology and give explanations on other influences.

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Multi-scale characterization of porous building materials

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X-ray computed tomography (X-ray CT) is one of the ideal tools to characterize the pore structure and matrix inside building materials such as open foam mortars. This technique is very useful for studying. It does not destruct the internal structure of the material and can directly obtain the spatial distribution of the pores and solid phase. The key purpose of this study is to obtain significant information about pore structure with X-ray computed tomography and 3D image analysis. 3D characterization will be used as input for further modeling (acoustic emission, fluid flow behavior). We will focus on the characterization of multiscale open foam mortars in order to extract their structural parameters which are key information for the understanding of their acoustic properties. Acoustical properties are those that govern how materials respond to sound waves, which are what we perceive as sound [1]. Acoustical properties are important parameters because open foam mortars have some it in that they will all absorb, reflect or transmit sound striking them. They can be acquired by using acoustic emission, which is a non-destructive method for examining behavior of the materials under investigation. Although this technique is easy to implement, the information gained is only global.

In order to establish a link between the macroscopic acoustic properties of the open foam mortars and the 3D microscopic characteristics, high resolution X-ray tomography will be perform at the Ghent University Centre of X-Ray Tomography (UGCT). We will set up a standardized workflow for the characterization of the multiscale open foam mortar. Additionally, fluid flow parameters such as open porosity, resistivity/permeability as well as mechanical parameters will be determined in lab. The multiscale 3D pore network will be used as input for acoustics simulation and laboratory measurements will be done to validate the simulated results. We will compare different procedures for mesh extraction and use relevant parameters for simulation. The combination of acoustic emission and micro-tomography imaging provides us with a unique opportunity to study acoustic emission in relation to the microstructure of the materials.

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Prediction of Archie's cementation factor by comparison study of electrical and hydraulic flow units, velocity deviation log and petrography

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Estimation of water saturation is one of the most important tasks in formation evaluation. The coefficients in Archie's equations are normally determined from laboratory data. Since carbonate rocks show drastic variations in lithology due to different texture and pore types, Archie's coefficients, which are more influenced by pore type, should be determined from different types of carbonate compared to constant values for a sandstone lithology. Uncertainties in these coefficients cause many errors in saturation evaluation, especially in case of oil in situ measurements. In this study different methods including petrography studies using thin sections and CT images, hydraulic and electrical flow units, and velocity deviation logs were compared to obtain Archie's coefficients (a and m). The results were compared to experimental measurements on numerous core plug samples, which have been taken from different types of carbonate reservoir rocks. The results show that the correlation coefficient between formation resistivity factor and porosity were improved by classification of samples using both texture and pore types (Hydraulic Units Delineation). Pore typing was done based on velocity deviation logs which are more accurate than the method using core data, density and neutron-density logs. Moreover the results were corrected by omitting low porosity samples in the evaluations where causes the improvement of the average correlation coefficients without low porosity samples from 80.8 to 88.8 percentage. Finally the results show that cementation exponent determined from electrical current units is more reliable than other methods that have been used in this study.

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Rare earth Chalcogels NaLnSnS4 (Ln= Y, Gd, Tb) for Selective Adsorption of Volatile Hydrocarbons and gases

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The synthesis and characterization of the rare earth chalcogenide aerogels NaYSnS4, NaGdSnS4 and NaTbSnS4 is reported. Rare earth metal ions like Y3+ , Gd3+ and Tb3+ react with the chalcogenide clusters [SnS4]4- in aqueous formamide solution forming extended polymeric networks by gelation. Aerogels obtained after supercritical drying have BET surface areas of 649 m2/g (NaYSnS4), 479 m2/g (NaGdSnS4) and 354 m2/g (NaTbSnS4). Electron microscopy and physisorption studies revealed that the new materials have pores in the macro (above 50 nm), meso (2-50 nm) and micro (below 2 nm) regions. These aerogels show higher adsorption of toluene vapor over cyclohexane vapor and CO2 over CH4 or H2. The notable adsorption capacity for toluene (NaYSnS4: 6.90 mmol/g), (NaGdSnS4: 12.36 mmol/g) and (NaTbSnS4: 9.76 mmol/g) and high selectivity for gases NaYSnS4 (CO2/H2: 155 and CO2/CH4: 37), NaGdSnS4 (CO2/H2: 172 and CO2/CH4: 50) and NaTbSnS4 (CO2/H2: 75 and CO2/CH4: 28) indicate potential future use of chalcogels in absorption-based gas or hydrocarbon separation processes.

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Scaling in hygromorphic response dynamics of wood

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Examples of wood products exposed to cyclically fluctuating relative humidity are abundant: furniture, flooring, structural elements, or art objects. The moisture content in such conditions changes continuously, which in wood is associated with expansion and shrinkage. This can lead to undesired effects, e.g. when the shape of an object changes, or in case of damage due to exceeding of the strength of the material by the associated stresses. It is therefore important to study the influence of moisture on the expansion of wood. Consider, e.g., the case of a panel painting, which consists of an oak board and paint on five of its six sides. When it is exposed to a change in the relative humidity at the non-painted surface, a non-uniform moisture content distribution over its thickness will lead to differential expansion. Macroscopically, the consequent bending moment will result in a curved board. Meanwhile, moisture transport takes place, resulting in a continuously changing moisture content profile, and thus a time-dependent curvature. Experiments and theory are presented in which this dynamic behavior is analyzed. A concise scaling law is presented, which is confirmed by experiments qualitatively, but not quantitatively. Since most objects in real-life applications are exposed to sinusoidal relative humidity fluctuations, the bending as a function of frequency is studied. It is shown that the bending follows linear system behavior, such that the frequency characteristics can be predicted by a simple experiment. The linear system behavior is also apparent from experiments with differently sized oak cubes, where the amplitude in moisture content and expansion is studied as a function of the frequency of relative humidity fluctuations. This provides a simple means of predicting the frequency behavior of wood objects with different dimensions.

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SELECTIVE COATINGGeneral Session FOR POROUS MEDIA COMBUSTION-BASED THERMOPHOTOVOLTAICS

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Thermophotovoltaic (TPV) systems represent an indirect, and potentially highly efficient, means to convert primary energy into electricity. These technologies can be designed as portable devices, which are able to provide high power density using a variety of heat sources, such as hydrocarbon fuel, solar, nuclear and waste heat. Moreover, efficiencies over 60% can (theoretically) be achieved in the case of high emitter temperatures, which makes this technology quite attractive for military, space, or any stationary/protable electrical generation applications [1]. The working principle of TPV technology is shown in Fig. 1. The concept is based on using an energy source to heat up an absorber/emitter material which then re-emits the energy towards the photovoltaic (PV) cells. With clever design it is possible to tune of the re-emitted spectrum to match with the PV cell's bandgap [2], i.e. releasing photons with energies higher than the bandgap energy level illuminate the PV cell. One of the major challenges of TPV systems is reducing the waste heat. A large portion of the input energy is typically wasted by convection in the flue gases. One potential way to create these temperatures involves using porous media combustion (PMC), due to the intense heat exchange from the combustion zone throughout the solid, enabling higher temperatures at outer (non-convective) surface of the solid matrix. To reduce un-useful radiative emission, the porous media matrix surface can be coated with a film to produce an emitter that matches to the spectral response to a GaSb PV cell, which has a bandgap energy at lambda_gap=1700 [nm]. In this work, we explore key low cost selective coating formulations over alumina (Al2O3) and silicon carbide (SiC) porous foam samples for this application. As such, different powders with selective emitter properties, such as erbia (Er2O3), ytterbia (Yb2O3), magnesium oxide (MgO) and nickel oxide (NiO) are spray and dip coated onto the porous mediums. Since these rare earth materials have a narrow emission bands at different excited state energy levels which are shown in Table 1 [3], it is hypothesised that they will serve as suitable selective emitters. In addition, a 2 wt.% NiO-doped MgO emitter at 1404 [°C] have shown a peak at 1400 [nm] [4]. Using an integrating sphere spectrophotometer, this study will measure total hemispherical reflectance to determine the emissivity of different combinations of these materials over the porous foams in order to have a coating with a high and broad emissivity in the range above the bandgap energy, but low emissivity beyond the bandgap. Finally, the findings of this research will inform and help the development of porous media-based TPV.

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Simulating CO2 and Tracer Transport in Cranfield Geological Carbon Sequestration Project with High-Resolution Static Models and an Accurate Equation of State

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Monitoring of natural (isotopic) and introduced tracers is a developing technology to further interrogate the subsurface for applications such as enhanced oil recovery and CO2 sequestration. In 2009-2010, a field-scale carbon dioxide (CO2) injection pilot project was conducted in a brine-saturated formation near Cranfield, Mississippi. Multiple perfluorocarbon tracers and isotopes were co-injected with CO2 and monitored at two observation wells. Surprisingly, tracer breakthrough at both monitoring wells occurred at nearly the same time, and was not significantly affected when the CO2 injection rate was nearly doubled. Multiple tracer peaks were also observed after breakthrough. These observations suggest that that multiple flow paths developed towards the monitoring wells. This is indicative of channeling through high permeability pathways formed by fluvial channels. The results demonstrate that tracers provide an important complement to transient pressure data. We present higher-order finite element simulations of the compositional two-phase flow during the experiment to better understand CO2 and tracer transport. High-resolution static models of the formation geology are used to capture the impact of connected flow pathways. Phase behavior is described by an accurate cubic-plus-association equation of state, which takes into account the polar nature of water molecules. Parameters studies are also presented that investigate the importance of Fickian diffusion, permeability heterogeneity, relative permeabilities, and capillarity.

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Storage feasibility in North Sea aquifers: Case studies from integration activities

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Carbon Capture and Storage (CCS) has a significant role for reduced CO2 emissions in Europe. According to the energy roadmap prepared by the EU Commission [1], emission reduction by CO2 storage amounts to average injection rates of 400 Mt/year until 2050. This can be compared to the North Sea Sleipner operation that has stored 1 Mt/year since 1996 in the Utsira formation. Large North Sea offshore storage formations of high quality are the likely major target for European emissions. However, an upscaling of today's injection rate by two orders of magnitude requires careful examination of injectivity, storage capacity and leakage risk. Several aspects deserve special attention, in terms of the physical system response, availability of data, and simulation techniques. Our simulation results show that pressure buildup is often the limiting factor for storage capacity. Although CO2 migration is limited to tens of kilometers near injection wells, the surrounding pore water can propagate the injection pressure pulse more than a hundred kilometers away. The magnitude of the overpressure is reduced with distance from injection wells, but parts of the aquifer that are closer to the surface have lower tolerance to overpressure. Therefore, the risk of caprock failure must be examined also in shallow regions far away from injection wells, and must include the post-injection period. In addition, the pressure tolerance may be further reduced in the presence of existing faults. The evaluation of storage feasibility is therefore pending on reliable data on formation depth, stress regime and presence of faults. In addition, the permeability, compressibility and porosity affect propagation of the overpressure and must be evaluated. Challenges then appear in terms of reliable data and simulation capabilities in formation volumes that can be an order of magnitude larger than those examined for hydrocarbon exploration. Data density is low for CO2 applications in untested aquifers, often with no core samples and unconfirmed seismic interpretations. In this work, experts on geology, geophysics, geomechanics, simulation technique and statistical analysis collaborate to optimize the use of existing data in an efficient simulation framework. Based on improved seismic

interpretation, analysis of formation tests, testing of wellbore cuttings and examination of leakage pathways, probability density functions are developed and used as input to simulations. The sensitivity of parameters and safe injection rates are evaluated based on a large number of simulations. The workflow is applied to the largest North Sea aquifer, the Skade/Utsira system, and to the Smeaheia formation where the aim is to store 1.5 Mt CO2/year, captured and transported from Norwegian onshore sources.

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Techno-Economical Study of near Miscible CO2 Injection in Candidate Carbonated Reservoir; CO2-EOR

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The main purpose of this investigation is to study the effect of near miscible CO2 injection on hydrocarbon recovery of the candidate carbonated reservoir and asses it both technically and economically. The economic study was done based on new Value Chain Analysis. In technical section, this effect can be traced by the change of two-phase gas-oil relative permeability curves. In this work, the experiments have been performed on three rock types (i.e. sandstone, dolomite, and artificial fractured sandstone) based on an incremental pressure algorithm approaching a near miscible condition. Lab-scale inverse modeling has been used to calculate relative permeability curves. Based on the experimental results, 85%of minimum miscibility pressure was defined as the near miscible pressure. Comprising the relative permeability curves in immiscible and near-miscible conditions shows that near miscible CO2 injection would be recommended in rock types with a lower RQI. Furthermore, in order to validate the lab scale results, the field scale modeling of the candidate reservoir was done using the 3D compositional reservoir simulator. The simulation results confirmed lab-scale data regarding the recovery factor in different rock types. In economic section, coupling of NPV analysis and value chain analysis is used as a strategic analytical and decision-support tool that created an added value regarding the higher oil production. To achieve this, comparison between two different strategies; including primary depletion and CO2-EOR was done to find the impact of CO2 on EOR. To reduce the uncertainty, sensitivity analysis was done on variables to find the optimum design parameters. The results show that with the detail lab and field study of CO2-EOR, higher oil recovery can be attained and this added value is economically profitable.

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The use of RFID technology to measure dielectric coefficients of diethyl ether-oil-brine mixtures for solvent enhanced imbibition experiments

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Description: Recent developments in ultra-high frequency (800MHz-1000MHz) Radio Frequency Identification RFID devices suggest that it is possible to use RFID for wireless laboratory measurements of the dielectric coefficients of fluid mixtures with possible spin-off for use in the petroleum engineering/ hydrology practice. This contribution demonstrates measurement of the dielectric coefficient of oleic and aqueous solutions of diethyl ether using a tag with dimensions 0.095 × 0.008 × 0.001 m3. As a precursor to the RFID measurements, we determined the concentration dependent partition coefficient, i.e. the ratio of the of diethyl ether concentrations in the oleic and aqueous phases, using an Anton Paar density meter. The phase behavior measurements are followed by simulations of the RFID setup in COMinisymposium OLTM to provide an understanding of the response dependence on the presence of the tag's encasement and the thicknesses of the blocks (media) surrounding the tag. Subsequently, we continue with the experiment of using a state of the art RFID device (RFID CISC Xplorer-2000) to examine the relation between RFID response and diethyl ether volume fractions in the oleic and aqueous phase. The measurements until now, however, show feasibility of using RFID technology to determine the diethyl ether water and diethyl ether-oil compositions.

Application: Concentration measurements in experiments for solvent enhanced recovery in fractured media.

Results, Observation, Conclusion: • Simulations with COMinisymposium OLTM help to improve the understanding of the tag's encasement and the dependency on the volumes of the media blocks covering the tag on both sides. • From the graphs where we plotted the RFID response functions versus the dielectric coefficient we can conclude that some frequencies indicate a larger dependence on the concentration (volume fraction) of diethyl ether in oil and diethyl ether in water than other frequencies. • Due to the strong dependency of the RFID response on the dielectric coefficient, the system can therefore be used for identification of dielectric coefficients.

Significant New Contributions: RFID technology can be used for wireless in-situ dielectric measurements and thus compositions in laboratory experiments in porous medium flow.

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Water Injection Performance Management as Investigation of Formation Damage by Injection and Production History

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Water injection is one of the process used in petroleum industry for improved oil recovery and pressure maintenance. The history of water injection is a cheap and useful tool to investigate well injectivities in lack of laboratory experiment during a water injection project. There are many easy-to-use techniques for monitoring a water injection /waterflooding, e.g. Hall plot and its derivative, WOR, GOR plots, instantainous and cumulative voidage replacement ratio (VRR), production heterogeneity index, scatter plot and etc. This paper tries to evaluate different excessive water production mechanisms such as near wellbore water channeling, rapid channeling and water coning and the effect of water injection on oil production of one of the Iranian oilfields using minimum available information of an injection and production well like injection pressure, injection rate, oil production rate, water production rate and the time period of injection by using the mentioned surveillance tools. In this research we use other techniques and data to compare results and Combination of techniques for better prediction.

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Applications of statistical mechanics to hysteretic capillary phenomena: ab initio predictions of contact angle on rough surfaces and of liquid retention in unsaturated porous media

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We describe a statistical mechanics approach to hysteretic capillary phenomena with two examples: the retention of a liquid in an unsaturated porous medium; and the behavior of the triple gas-solid-liquid contact line on a rough surface. In both cases, random geometry of pores or cavities produces a frozen disorder that is subject to the collective release of capillary energy in first-order phase transitions. In unsaturated porous media, this may lead to Haines jumps. For the advancing and receding contact line, the analysis predicts six distinct regimes that include the classical Cassie-Baxter state, metastability, and other behavior observed in experiments. The first graphic illustrates how the geometry of a microscopic bed of rods produces such wide variety of hysteretic contact angle behavior; the second shows how retention curves are affected by the statistical distribution of specific pore area and necks cross-section in unsaturated porous media.

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Continuum Approach in Modelling and Simulations of Ceramic Manufacturing Processes

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This talk will focus on integrating material parameters with transport phenomena during ceramic manufacturing, and how they can be used to create models to describe the effect of material, shape configuration and process parameters on the final quality of the produced parts. The simulations are tailored to address ceramic flow in the tape casting process. Tape casting has been used to produce thin layers of ceramics that can be applied as single layers or can be stacked and laminated into multilayered structures [1]. A tape layer can be considered as a porous medium which contains powders and liquid phases. The distribution of particles inside the ceramic slurry will affect the topology of the pores and their distribution, which in turn will influence the subsequent drying process of the ceramic layers. With this in mind, examples of flow simulations in tape casting will be discussed and compared with experimental results [2]. Finally, the impact of intrinsic material properties, process parameters, as well as the configuration of the layered structure on the drying behavior of the ceramic layers will be highlighted [3].

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Mathematical Modelling of Mechanical Dewatering of a Paper Web inside a Press Nip

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The process of papermaking may be regarded as a dewatering and drying process, during which the paper web is transported directly or supported by a permeable fabric through single aggregates, e.g. former, press or dryer. The dewatering and drying behavior defines significantly the properties and quality of the final product. Modeling and simulation of the process steps involved offer insights into the mechanisms of water removal and sheet construction, which cannot come from measurements and experiments alone and thus give new impulses that can directly be used to improve and redesign processes and components. We present a modeling approach of a press nip, where the essential part of the mechanical dewatering of the paper web takes place. Dewatering is achieved by applying high mechanical load to the wet paper web using two opposing rolls. The high pressure causes a flow of water from the paper through a press felt into the open surface space of the underlying roll cover. Thus, the dewatering process in the press section can be described by a simultaneous two phase flow of water and air though the porous media paper web, felt and roll cover. In addition, the compression of both the paper web and the press felts has to be taken into account. The dewatering process in the press nip includes different length and time scales that span multiple orders of magnitude enforcing the simulation to follow a multiscale approach. We use high-accuracy tomographic imaging together with other lab data and fast and efficient numerical methods to study the mechanical and the fluid dynamical properties of the fiber web and paper machine clothing. With these small scale simulations we obtain the effective parameters describing the important aspects of the materials involved in the dewatering process. These effective material models are then used to model and simulate dewatering inside the press nip.

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Multiscale imaging and upscaling using machine learning

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We present a technology that combines imaging techniques with machine learning to characterize multi-scale rock properties. The technology is based on the understanding that a rock consists of building blocks, i.e. fabrics, intermixed spatially at various scales. Detailed knowledge of all fabrics at its representative scale will lead to an improved characterization of the rock sample. A fabric possesses a set of properties, e.g. porosity, fraction of organic matter, pore size distribution and others. Unsupervised machine learning is used to learn about fabrics present in a sample. It also recommends optimum sub-sampling areas for smaller-scale higher resolution image acquisition and properties upscaling. The required resources in this approach are several orders of magnitude lower than acquiring mosaics of small-scale images covering a similar area at the large scale. We apply the present technology to acquire images and characterize pore properties of rock samples from Eagle Ford, Marcellus and Wolfcamp. The rock sample area is approximately 0.5 x 0.5 [mm] with a resolution of 244 [nm]. Small-scale images with an area of approximately 30 x18 [micron] with a resolution of 10 [nm] are used to characterize pores within fabrics. The upscaled pore properties and fractions of organic matter are compared with that derived from small-scale mosaic covering a similar area. The comparison shows a very good agreement confirming the accuracy and reliability of the present technology.

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Seismicity-Permeability Coupling in Porous and Fractured Media

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Contemporary methods of energy conversions that reduce carbon intensity include sequestering CO2, fuel switching to lower-carbon sources, such as from gas shales, and recovering deep geothermal energy via EGeneral Session . In all of these endeavors, either maintaining the low permeability and integrity of caprocks or in controlling the growth of permeability in initially very-low-permeability shales and geothermal reservoirs represent key desires. At short-timescales of relevance, permeability is driven principally by deformations – in turn resulting from changes in total stresses, fluid pressure or thermal and chemical effects. These deformations may be intrinsically stable or unstable, result in aseismic or seismic deformation, with resulting changes in permeability conditioned by the deformational mode. We report experiments and models to represent the respective roles of mineralogy, texture, scale and overpressures on the evolution of friction, stability and permeability in fractured rocks, and their consequences on fluid production, containment and induced seismicity.

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Understanding Transport Processes in Thin Porous Electrodes of Electrochemical Devices via X-ray Computed Tomography

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Understanding transport processes in thin porous carbon materials is critical for electrochemical energy applications. However, tools that are designed for characterization of porous media on a large scale are not always applicable for thin (< 500 um) layers. Moreover, it is essential to bridge nano- and micro-scale transport processes, as fine nano-structures of carbon materials are desirable for high surface area and the features of a larger size are needed for high hydraulic permeation. To characterize transport on nano and micro-scales synchrotron X-ray computed tomography (CT) is well-fit due to its fast, non-intrusive measurements that allows quantification of morphological properties of porous media. For polymer-electrolyte fuel cells (PEFCs) and anion exchange membrane fuel cells (AEMFCs) effective water management remains a hurdle, especially at lower operating temperatures. During start-up and operation liquid water formed as a byproduct of electrochemical reaction can block gas (reactant) delivery to a catalyst, resulting in flooding, mass-transport losses, and low cell power densities. Using synchrotron X-ray CT we have previously shown morphology and transport dependencies on material structure, compression and chemical composition.1, 2 These ex- and in-situ studies are useful and shed light on an isolated transport phenomena. Continuum, pore-network and direct meshing models are used to explain the observed phenomena and to guide the fuel cells components design.3, 4 Addressing and understanding water transport issues, however, is made possible by introducing the capabilities for in-operando X-ray CT. In this presentation in-operando steady-state water distribution will be shown in PEFCs and AEMFCs for temperature of 30oC with chronoamperometric holds. Furthermore, comparison of water distribution in platinum group metals (PGM) and PGM-free catalysts for both type of fuel-cells will be presented. In all of these examples liquid water pooling was observed at the component interfaces, where larger voids were present.

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A Hierarchical Finite Element Monte Carlo Method for Stochastic Two-Scale Elliptic Equations

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We consider two-scale elliptic equations whose coefficients are random. In particular, we study two cases: in the first case, the coefficients are obtained from an ergodic dynamical system, and in the second the case, the coefficients are periodic in the microscale but are random. We suppose that the coefficients also depend on the macroscopic slow variables. While the effective coefficient of the ergodic homogenisation problem is deterministic, to approximate it, it is necessary to solve cell problems in a large but finite size “truncated” cube and compute an approximated effective coefficient from the solution of this equation. This approximated effective coefficient is, however, realisation dependent; and the deterministic effective coefficient of the homogenisation problem can be approximated by taking its expectation. In the periodic random setting, the effective coefficient for each realisation are obtained from the solutions of cell problems which are posed in the unit cube, but to compute its average by the Monte Carlo method, we need to consider many uncorrelated realisations to accurately approximate the average.

Straightforward employment of finite element approximation and the Monte Carlo method to compute this expectation with the same level of finite element resolution and the same number of Monte Carlo samples at every macroscopic point is prohibitively expensive. We develop a hierarchical finite element Monte Carlo algorithm to approximate the effective coefficients at a dense hierarchical network of macroscopic points. The method requires an optimal level of complexity that is essentially equal to that for computing the effective coefficient at one macroscopic point, and achieves essentially the same accuracy. The method combines the hierarchical finite element method for solving cell problems at a dense network of macroscopic points with the optimal complexity developed in D. L. Brown, Y. Efendiev and V. H. Hoang, Multiscale Model. Simul. 11 (2013), with a hierarchical Monte Carlo sampling algorithm that uses different number of samples at different macroscopic points depending on the level in the hierarchy that the macroscopic points belong to. Numerical examples confirm the theoretical results.

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A pore scale model for osmotic flow: homogenization and lattice Boltzmann simulations

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On a macroscopic level, the process of osmosis is well understood. The transport of solvent and solute across a semi-permeable membrane is described by the Kedem-Katchalsky equations

for the respective fluxes J_v and J_D driven by the hydrostatic pressure difference \Delta p and the concentration difference \Delta c. At steady-state, there is a balance of the hydrostatic pressure and the osmotic pressure

where \sigma is the so called reflection coefficient, which is related to the parameters L_p and L_{pD} above.

However, at the pore scale of a porous medium, it is less clear what the correct model should be, and several theories have been proposed over the years. Here, we present a general microscopic model including osmotic effects in the Stokes' and advection-diffusion equations [1]. The model agrees with Anderson and Malone's model for straight cylindrical channels [2], but is a full 3D model.

Additionally, we present homogenization results for this system in a periodic porous medium [1], showing how the parameters of the Kedem-Kachalsky equations can be computed from the local cell problem. In particular, a method to compute the reflection coefficient \sigma from the local material properties is shown. The model has also been implemented using the lattice Boltzmann method, and results are shown both for the full microscopic model and for computations of \sigma for a selection of porous medium geometries.

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Computational investigation of a novel porous media phase field equation: convergence and coarsening rates

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We study interfacial dynamics in strongly heterogeneous domains such as porous media based on Cahn-Hilliard/Ginzburg-Landau phase field equations. To systematically account for the pore geometry, we use the recently derived homogenized formulation [1,2,3]. We compare numerical solutions of the microscopic formulation fully resolving the pore space with the upscaled/homogenized porous media formulation [2]. For circular pore-walls we validate the rigorously derived convergence rate $\mathcal{O}(\epsilon^{1/4})$. In the case of square shaped pore-walls, the convergence rate improves to $\mathcal{O}(\epsilon^{1})$. A computation of the homogenization error over time for different pore geometries shows a complex interplay between pore geometry and heterogeneity. Finally, for both, the homogenized and the microscopic formulations, we recover the experimentally validated and rigorously derived coarsening rate $\mathcal{O}(t^{1/3})$ in the periodic porous media setting.

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Different scaling regimes for modeling and simulation of reactive transport in 3D porous media

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Pore-scale modeling and simulation of reactive flow in porous media has a huge range of diverse applications, and poses a number of research challenges. It is known that the morphology of a porous medium has significant influence on the local flow rate, which can have a substantial impact on the rate of chemical reactions. While there are a large number of papers and software tools dedicated to simulating either fluid flow in 3D computerized tomography (CT) images or reactive flows using pore network models, little attention to date has been focused on pore-scale simulation of surface reactions in 3D CT images. In this talk we will present an asymptotic analysis of the reactive transport through a porous medium, with chemical reactions taking place on the pore surfaces. The Peclet number is expressed as a negative power of the dimensionless characteristic pore scale epsilon. The observation time is the characteristic global advection time scale and it is compared with the superficial chemical reaction time scale, with characteristic adsorption/desorption times and with Peclet's number. Due to the complex geometry and in presence of dominant Peclet and Damkohler numbers, solving the full problem for arbitrary values of coefficients is costly and practically impossible. Consequently, we apply homogenization to find the effective (or averaged or homogenized) values of the dispersion coefficient and the transport velocity and an effective corresponding parabolic equation for the effective concentration, valid in every point of the porous medium.

The scalings of interest for the Peclet number Pe are i) Pe =O(1) and ii) Pe=O(1/ epsilon). We couple it with appropriate scalings for the ratios of other characteristic times with the superficial chemical reaction time scale. Using the techniques developed in [1], [2] and [3], different upscaled models are derived. Calculating effective coefficients (the dispersion coefficient, memory effects, ..) in 3D pore geometries requires robust algorithms for the simulation of such reactive flows directly on images, which is implemented in a sophisticated software package. This software is then used to present numerical results for several nonlinear isotherms in two separate resolved geometries.

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Effective reaction and deposition rate in periodic sphere packings

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In the upscaling from pore- to continuum (Darcy) scale, reaction and deposition phenomena at the surfaces of a porous medium, have to be represented as macroscopic reaction source terms. The effective rates can be computed, in the case of periodic media, from three-dimensional microscopic simulations of the periodic cell. Several computational and semi-analytical models have been studied in the field of colloid filtration to describe this problem. Most of them, however, rely on effective deposition rates defined by simple linear reaction ODE, neglecting the advection-diffusion interplay. These rates are then inserted into general macroscopic transport equations, leading to a conceptual inconsistency and, therefore, often qualitatively wrong results. In this work, we study the upscaling limit of ideal deposition in BCC and FCC spherical arrangements using a formal volume-averaged and homogenised effective reaction rates, in the fast reaction limit. We make use of a particularly convenient computational setup that allows us to compute directly the asymptotic stationary value of effective rates, exploiting the linearity of the equation, in contrast to most of the existing approaches that typically neglects the existence of a transitory solution that, depending on the Peclet number, typically vanishes after a few unit cells. We show how this new definition of deposition rate is more robust and extendible to the whole range of Peclet numbers and it is consistent with the macroscopic model of interest. Possible extensions to non-linear equations are discussed.

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Extreme localisation property for eigenfunctions of one-dimensional high-contrast periodic problems with a defect

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Following a number of recent studies of resolvent and spectral convergence of differential operators describing the behaviour of periodic composite media with high contrast, we shall discuss the corresponding one-dimensional version that includes a ``defect'': an inclusion of a fixed size with a given set of material parameters. We show that the eigenvalues of the related operator in the space of square integrable functions converge to points of the spectrum of a limit operator whose continuous spectrum has a band-gap structure. In cases when a limit eigenvalue is situated in a gap of the continuous spectrum, this leads to the existence of a wave propagating along the defect and extremely localised in its neighbourhood.

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Flow Through Porous Media: a Momentum Tracer Approach

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The flow of a fluid through a spatially periodic porous medium is studied using the momentum tracer approach, that is by monitoring the temporal spread of an instantaneous source of momentum (the ''momentum tracer''), following its initial introduction into the interstitial fluid. The fluid flow is described macroscopically by a Brinkman-like effective equation, containing three effective tensorial quantities, namely the permeability dyadic, the generalized viscosity tetradic and a coupling triadic term. These phenomenological coefficients are shown to be expressible in terms of the solution of the characteristic eigenvalue problem associated with the (tensorial) Stokes operator, defined within the interstitial region of a single unit cell of the periodic porous medium. The phenomenological coefficients are shown to be independent of the initial position of the momentum tracer as well as of the choice of weight function used in averaging the microscale momentum density over the unit cell. Finally, we show that the analytical expressions for the phenomenological coefficients identically satisfy the symmetry requirements that can be obtained by applying the reciprocal theorem at the macro-scale level.

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Homogenisation using energy decomposition

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In this talk, we discuss a homogenisation approach based on decomposing the solution space into slow and fast components. Such a decomposition allows one to reformulate the energy minimisation problem related to a given PDE as minimisation over slow and fast component. The fast minimisation problem can be approximately solved as a function of the slow component. Due to our construction of the fast space, this minimisation problem can be solved locally. In the linear periodic setting this leads to the well known cell problem.

The approach presented in this talk allows one to analyse the error in the homogenised solution using perturbation arguments. Working in perturbation setting is well motivated, as a vast majority of convergence estimates found in numerical analysis are either perturbation or projection type. An outline of a convergence proof will be given for a linear material with rough material parameters. To illustrate the wide applicability of the method, numerical examples are given in 2D from stochastic homogenisation, homogenisation of domain with holes and homogenisation of a non-linear problem.

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Homogenization of Thermoelasticity Processes in Media Undergoing a Priori Known Phase Transformations

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Steel can be seen as a porous media with extremely active microstructures (especially if they are thermally excited) and is known to exhibit a complex material behavior where the macroscopic properties are highly dependent on the underlying microstructures. The medium in question consists of a connected matrix with disconnected, initially periodically distributed inclusions separated by a sharp interface undergoing an a priori known interface movement due to phase transformations. For the resulting linear, fully coupled thermoelasticity problem, we investigate well-posedness and a priori estimates. Via a two-scale convergence argument, we then show that the epsilon-dependent solutions converge to solutions of a corresponding upscaled model with distributed time-dependent microstructures.

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On Permeability Dynamics in Carbonaceous Aquifers used in Energy Storage Applications

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Geothermal energy harvesting applications use deep groundwater aquifers to store harvested energy. The impact of this additional energy to the aquifer chemistry is crucial for long-term operation. Gaseous CO2 is added to the injected water to compensate potential precipitates of carbonates and to prevent structural changes to the aquifer. Both of these effects affect the local chemical equilibrium of the aquifer, and we consider an effective model through homogenization which captures the hydrochemistry, heat transfer, fluid flow and permeability dynamics of the aquifer as heated fluid is added to the aquifer (injection), and as it is later removed (production). The impact of these different physical mechanisms of the heat storage performance of the aquifer is discussed.

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Phase-field fracture propagation in porous media

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In this talk, we present modeling and numerical simulations of fracture propagation in porous media using a phase-field technique. A smoothed indicator function determines the crack location and is characterized through a model regularization parameter. In addition, modeling assumes that the fracture can never heal, which is imposed through a temporal constraint, leading to a variational inequality system. For reliable numerical simulations, key aspects are robust and efficient algorithms for imposing the previously mentioned crack irreversibility constraint, treatment of the indefinite Jacobian matrix, and local mesh adaptivity for a high mesh resolution of the fracture zone. As applications, we focus on multiphysics phase-field fracture such as pressurized fractures and fluid-filled fractures in porous media that include achievements as well as current limitations.

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Quantitative stochastic homogenization: Recent advances and perspectives

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In recent years, the quantitative stochastic homogenization of linear diffusion equations has seen tremendous progress: In particular, for the first time optimal estimates for the homogenization error - that is, the error caused by replacing the microscopic model by the macroscopic homogenized equation - have been derived by Gloria and Otto and by Armstrong, Kuusi, and Mourrat. We provide an overview of the recent advances and outline future perspectives concerning the quantitative homogenization of transport equations and related models associated with random porous media.

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Sequential homogenization of reactive transport in polydisperse porous media

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We investigate the applicability conditions for sequential homogenization of reactive solute transport in bi-disperse porous media. We consider reactive solute transport in a fully saturated porous medium constituted by an array of periodic meso-scale rigid obstacles embedded in a permeable porous matrix with different surface reactivity. The geometric characteristics of the system can be described by two separation of scale parameters. The dispersion coefficient and effective reaction rate of the physically and chemically bi-disperse medium can be obtained by sequential homogenization. In contrast with classical one-step homogenization, sequential homogenization is performed through iterations of multiple-scale expansions, starting from the smallest scale. Iterations are more computationally efficient, but, in general, less accurate. Beside truncation errors, the iterations introduce additional errors due to the quasi-periodicity of the porous matrix. Specifically, the error is inversely proportional to the number of non-periodic "unit cells" along the surface of the obstacles. We show that under appropriate conditions, expressed in terms of the Péclet number and the scales separation parameter, second order accuracy of the sequential upscaling method can be achieved.

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Stochastic homogenization of rate-dependent systems in plasticity theory

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In this work we are concerned with the stochastic homogenization of the initial boundary value problems of monotone type. The models of monotone type under consideration describe the deformation behaviour of inelastic materials with a microstructure which can be characterised by random measures. Based on the Fitzpatrick function concept we reduce the study of the asymptotic behaviour of monotone operators associated with our models to the problem of the stochastic homogenization of convex functionals within an ergodic and stationary setting. The concept of Fitzpatrick's function helps us to introduce and show the existence of the weak solutions for rate-dependent systems. The derivations of the homogenization results presented in this work are based on the stochastic two-scale convergence in Sobolev spaces. We present also the convergence results, which are related to the classical Γ-convergence results.

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Upscaling reactive ion transport under dominant flow conditions

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Investigating flow and transport in porous media is a classical multi-scale problem. In recent research, upscaling approaches have been undertaken for models integrating electrostatics or deformations of the porous matrix resulting from chemical reactions, among others.

In this presentation, we consider reactive ion transport under dominate fluid flow conditions in a thin, potentially evolving, strip. Electric charges and applied electric potentials (e.g. zeta potential) give rise to electroosmotic flow in addition to pressure driven flow. At the pore-scale a mathematical model in terms of coupled partial differential equations is introduced. It consits of a transport equation (convection-diffusion-drift-reaction-equation) for mobile, charged, chemical species, Stokes equations for the fluid flow, and Poisson equation for the electrostatic potential. In the chosen geometrical setting, the free boundary, i.e. the interface between the attached layer of immobile chemical species and the fluid is described via the thickness of the layer. To this model, a formal limiting procedure is applied. Discussing the upscaled model we focus on dispersive effects that occur under the applied dominant flow conditions. In doing so, we focus on the difference and also interplay of hydrodynamic dispersion (Taylor-Aris dispersion) and dispersion created by electroosmotic flow.

The theoretical results are complemented by numerical computations for the different settings. A thorough parameter analysis is conducted related to pressure and electroosmotic terms.

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A Review on Enhancing Heat Transfer Processes by Open-cell Metal foams and Industrial Applications

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In last couple of decades researchers' attitudes were focused on developing and enhancing heat transfer processes by using new components or cellular solids that divides in: stochastic structures and periodic structures. Open-cell metal foams are part of stochastic structures families that they can be considered as a avant-garde technology and they have unique properties, this porous media can have tremendous achievements in thermal processes. This paper argues and surveys postulating possible in industrial thermal issues. Includes: compact electronic cooling, heat exchanger, areo space, fines, turbo machineries, automobiles, crygen tanks, biomechanics, high temperature filters and etc.Recently by surveying exponential publications rate in thermal open-cell metal foams issues , it can be demonstrated a holistic view which can lead researchers to a new level of understanding in different industrial thermal sections.

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Asymptotic modelling of multi-dimensional jump conditions at a fluid-porous interface

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This work proposes an asymptotic modelling (Angot 2003, 2011) of multi-dimensional unsteady viscous fluid flow and heat or mass transfer at a fluid-porous interface. The asymptotic analysis is developed considering that the thickness d of the interfacial tran- sition region Ωfp in the one-domain continuous representation is thin compared to the macroscopic length scale of the system L. Thus, a two-domain model is obtained where the averaged mass, momentum or heat transfer in the transition layer are replaced by algebraic jump boundary conditions at a fictive dividing interface Σ separating the homo- geneous fluid and porous regions. These interface conditions for the jumps across Σ of the stress and velocity vectors, or heat flux and temperature, are stated up to first-order in O(d/L). The resulting original fluid-porous asymptotic model is then described either by the Stokes and Darcy or Darcy-Brinkman equations coupled with the advection-diffusion- reaction of heat or mass transfer and supplemented with the present jump conditions at the interface. Due to its multi-dimensional character, this new asymptotic model is found to be very attractive and general. Indeed, all the existing fluid-porous interfacial jump conditions, generally restricted to the 1-D channel shear flow (Beavers & Joseph 1967; Ochoa-Tapia & Whitaker 1995; Valď es-Parada et al. 2013) are recovered by taking the tangential component of the asymptotic jump conditions. This comparison gives explicit expressions of the effective jump coefficients and the definition of their associated scaling. Another important result is that the asymptotic model allows us to derive a new equa- tion for the pressure jump which does not vanish a priori as soon as there is a non-zero transverse flow at the interface.

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Bubble Formation and its Effect on Interfacial Area Evolution and Topology in Two-Phase Flow

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The use of macro- and nano- bubbles for use in environmental engineering applications (e.g. air sparging of gasoline contaminated aquifers and dissolved oxygen enhancement in bioremediation efforts) has shown great potential in the past few years. As this technology gains more attention, the modeling of the transport aspects of bubbles in porous media becomes important [1]. In multi-phase flow, bubble transport could influence flow paths in the porous medium and, therefore, need to be accounted in multi-phase flow models. One such multiphase flow theory introduces thermodynamically derived specific interfacial area as a state variable to better describe the system by reducing or eliminating the hysteric effect prevalent in conventional capillary pressure-saturation relationships that model two-phase flow [2]. If bubbles become trapped in pores or incorporated in another gas phase (adding to specific interfacial area) a capillary pressure-saturation-specific interfacial area (Pc-Sw-Anw) relationship might not fully capture the history of the system. We will present an analysis of the uniqueness of the Pc-Sw-Anw and relationship under normal two-phase flow conditions and with bubble formation from data collected using dynamic x-ray microtomography.

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DYNAMICS OF PORE-FILLING AND SNAP-OFF EVENTS DURING IMBIBITION IN CARBONATE ROCKS

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We have investigated the pore-scale mechanisms of oil trapping during brine invasion in carbonate rocks, under capillary-force dominated flow and reservoir pressure conditions. To image the dynamics of the brine-oil front progression and snap-off process, real-time tomograms with a time resolution of 38 s (24 s for imaging and 14 s for recording the data) and a spatial resolution of 3.28 µm were acquired using synchrotron X-ray tomography. From the analysis of the local capillary pressure, calculated from the brine-oil interface curvature maps, we quantify the conditions under which a pore-filling event and snap-off occur. We show that a significant decrease in the local capillary pressure on the ganglion-side connected interfaces causes a local pressure gradient resulting in the migration of brine towards an adjacent throat (brine layer swelling), until a capillary threshold pressure is reached and the brine-oil interface becomes unstable resulting in the snap-off of the oil phase. We have also investigated various pore morphologies in which snap-off occurs, i.e., between two throats and at a junction of three pores/throats. We further analyze the pore-filling (by brine) event sizes, which indicates an increase in the volume of the largest event (between consecutive images) with time (or injected pore volume). This is linked to a decreasing capillary pressure with time, resulting in the invasion of larger pores with time. Although, the maximum size of an event is about an order of magnitude larger than the average pore size, we show that the pore-filling events do not cascade over multiple pores, and therefore, pore-scale inertia is not needed in explaining a capillary-force dominated flow regime during imbibition.

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Effects of temporal fluctuations on mixing of two fluids for a stable stratification

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Mixing and dispersion in aquifers are controlled by concentration gradients which are strongly influenced by periodic temporal flow fluctuations on multiple time-scales ranging from days (tides), seasons (pumping and recharge) to glacial cycles (regression and transgressions). We study effective mixing and solute transport in temporally fluctuating one-dimensional flow for a stable stratification of two fluids of different density. The impact of the fluctuations on the interface between the two fluids is characterized by the spatial moments of the gradient of the solute concentration distribution and quantified by the evolution of the variance of the gradient distribution. An effective time-average formulation is derived to describe the coupling between mixing and oscillatory transient flow under nonstationary flow conditions. Explicit expressions for the concentration distribution and the variance are developed to predict the transient mixing dynamics. We find that the magnitude of transient-driven mixing is mainly controlled by the hydraulic diffusivity, the period, and the initial interface location. We also identify two dominant regimes in the temporal evolution of the variance in response to the spatial and temporal variability of the velocity field induced by temporal fluctuations. At small times, the width of the mixing zone is mainly influenced by the flow velocity at the interface location and both the center of mass as well as the variance increase linearly with time. For increasing times, the spatial variability of the flow velocity leads to a deceleration of the interface and a compression of its width which results in a logarithmic upward displacement of the center of mass and a subdiffusive growth of the variance with t$^1/2$. Detailed numerical simulations and as well as accurate column experiments under well-controlled laboratory conditions are presented to validate the theoretical effective model defined. The proposed formulation is found to provide very good predictions and correctly reproduces the mixing dynamics.

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Emulsion Flow in Different Wettability Pores Studied using 4D Image Analysis

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The flow of emulsions through porous media is fundamental in the development of enhanced oil recovery processes. In this work, we evaluate the impact of different emulsion stabilization mechanisms on the stability of emulsion flow through model pores of different wettability. Specifically, we study the impact of surfactant versus nanoparticle stabilization or combination nanoparticle/surfactant systems with different excess components (e.g. excess surfactant or nanoparticles with different interfacial adsorption properties) on the stability of emulsions during flow. Remarkable deviations from simple translational flow are observed depending on the compatibility of the emulsifier(s) with the pore wall. Flow instabilities were primarily examined using 4D laser scanning confocal microscopy imaging, which allows for both the emulsion droplets and nanoparticle emulsifiers to be directly imaged in real time during flow through the model pore system. In conjunction with bulk instability analysis (e.g. extent of coalescence after flow of a specified volume through the model pore), 4D image analysis enables a fundamental understanding of the mechanisms governing the observed flow instabilities. Combination nanoparticle/surfactant systems are demonstrated to exhibit the greatest stability due to an apparent “shielding” behavior by the excess emulsion stabilizers, which prevents the droplets from experiencing incompatibilities with the pore wall to the full extent.

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Estimating critical curvatures for pores of heterogeneous wettability

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Understanding of pore-scale physics for multiphase flow in porous media is essential for accurate description of various flow phenomena. In particular, capillarity and wettability strongly influence capillary pressure-saturation and relative permeability relationships. Wettability is quantified by the contact angle of the fluid-fluid interface at the pore walls. In this work we compare a popular open-source finite volume computational fluid dynamics solver with a new formulation of the level set method that models quasi-static capillarity-dominated displacement and is therefore less computationally expensive. The methods fundamentally differ in the way they capture interfaces, as well as in the number of equations solved and other implementation and algorithmic details. Both methods are able to solve curvature-driven displacement and implement arbitrary contact angles at pore walls. The methods are tested in rhomboidal packings of spheres for a range of contact angles and for different rhomboidal configurations. Predictions are validated against the semi-analytical solutions obtained by Mason and Morrow (1994). We evaluate the benefits and limitations of employing a less computationally intense method for semi-equilibrium capillary-dominated flows vs. the full approximation of the Navier-Stokes equation - also applicable to inertial and viscous flows. Finally, we show critical curvature results in fractionally wet pores (with varied spatial arrangements of grains of different wettability) for which we do not have analytical solutions.

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Experimental study of relative permeability and saturation variations in a fractured basalt core

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Large sedimentary basins have been shown to have significant capacity to store CO2 that has been captured from power plants or other industrial sources. However, there are many locations with large CO2 emission sources that are not located close to sedimentary basins. Under these conditions, storage in basalt rocks may provide an alternative. Basalt rocks are not only abundant, enormous volumes of mafic and ultramafic rocks are present on the Earth's surface, but also have shown a greater potential for mineral trapping. Fluid flow in basaltic rocks is governed by the permeable paths provided by rock fractures. If the CO2 can react with the basaltic rocks to form stable minerals before it leaks up these fractures, storage in basaltic rocks may provide a viable alternative to storage in sedimentary basins. Flow through fractures has been a focus of research for decades but there are still some gaps in experimental knowledge related to fracture aperture distributions and permeability stress-dependency: How do fracture aperture and relative permeability variations influence CO2 injection? What are the implications of permeability stress dependency? How do the changes of the liquid-gas interface affect relative permeability? Previous studies show contradictory results and difficulties to measure such variables (Huo and Benson, 2016). In this study, multiphase core-flooding experiments are conducted to address these questions. We use X-Ray CT imaging to calculate fracture aperture and saturation distributions. While the aperture distributions can be determined quite accurately, even for fractures as small as ~30 micron, other parameters are more difficult to measure. Here we focus on the experimental challenges associated measuring fluid saturations using X-rays and uncertainty with regard to the fluid phase the pressures are being measured in. Consequences of these uncertainties on the reliability of the measurements are presented. We provide new experimental data from natural and manmade fractures in basalt cores. In addition, we reinterpret previous experiments in fractured cores based on new insights about measurement techniques.

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Fluctuating interfaces in disordered media and their macroscopic representation

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We study the evolution of interfaces in disordered media starting from stochastic representations of the microscopic interface dynamics in terms of the Edwards-Wilkinson (EW) and Kadar-Parisi-Zhang (KPZ) models [1]. The EW and KPZ approaches describe the evolution of a fluctuating interface as the competition of interface smoothing due to fluid viscosity and mass transfer perpendicular to the growth direction and stochastic fluctuations as a result of spatial and temporal disorder. While the KPZ model has been used to classify and quantify the evolution of pore-scale fluid interfaces in, it has not been known, which are the consequences of the KPZ relaxation-fluctuation dynamics on the Darcy-scale phase saturation dynamics. In this framework, the phase saturation at a given position is obtained by a cross-sectional average of the interface indicator, which counts 1 behind and 0 in front of the interface, see Figures. In order to derive the (deterministic) saturation dynamics, we first determine the one-point interface height statistics for the EW and KPZ models. While we obtain exact results for the EW model, we develop a Gaussian closure approximation for the KPZ model. This yields an explicit evolution equation for phase saturation. We identify an interface compression term, which is related to mass transfer perpendicular to the growth direction, and a diffusion term that tends to increase the interface width. The interface compression rate depends on the mesoscopic mass transfer process along the interface and in this sense provides a relation between meso- and macroscopic interface dynamics. These results shed light on the relation between mesoscale and macroscale interface models, and provide a systematic framework for the upscaling of stochastic interface dynamics [2].

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Interfacial Curvatures and Nonwetting Phase Trapping for Two- and Three-phase Flow in Porous Media

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We use x-ray microtomography images to predict capillary pressure via interfacial curvature measurement for both two- and three-phase fluid porous media systems.

The data allows us to separate connected and disconnected phases in the images, and thereby track the pressure state of both connected (bulk) and disconnected (trapped) nonwetting phase. For both two-phase and three-phase flow, the pressure state of disconnected non-wetting phase is bound by the pressure state of the bulk fluid, i.e., the Pc-S curve for disconnected phase exists within the connected Pc-S curve branches, meaning that the disconnected blobs must adhere to points along scanning curves for the bulk fluid.

The data also suggests flow through films as a conduit of nonwetting phase flow between connected (bulk) fluid and seemingly disconnected phase. Individual objects can be followed during several drainage and imbibition cycles, and curvature changes followed as the pressure state of an apparent disconnected blob adjusts to the pressure of - and equilibrates with - the energy state of the bulk fluid via film flow. This has important implications for how we understand trapping in multi-phase porous medium systems and highlights the potential importance of flow in films with a thickness below the image resolution.

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Mixing in a Vapour-Vapour-Liquid system: Microfluid Oberservation During SC-CO2 Displacing Condensate Gas With High Temperature

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Vapour-Vapour-Liquid three phase reservoir conditions (high temperature) have been created using a microfluid system to understand the effect of supercritical CO2 on the phase behavoir peroperties of gas-condensate hydrocarbons. Novel phase behavior experimental procedures and phase equilibrium evaluation methodology for gas-condensate phase system mixed with supercritical CO2 with high temperature have been presented. A unique phase behavior phenomena was also reported. In our experiment, When pressure drop to specific pressure range, the interfacial phenomena between condensate gas and supercritical CO2 like fine mist or cloudiness appeared in PVT cell were observed and recorded. The thermodynamic properties of different vapour phases were measured. Another important observation is the mass transfer of supercritical CO2 into the condensate gas. The mass transfer time between two vapour phases was also measured. Experiments verify that under a certain pressure and CO2 concentration conditions with high temperature, supercritical CO2 can be used as efficient displacing media to flood condensate gas, where CO2 displacing behavior looked like “cushion gas” and CO2 was not easy to be mixed with condensate gas.

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Model based domain decomposition methods for partially saturated flow in porous media

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Aside from physical accuracy of the models, computational problems around groundwater flow, comprise manifold hallenges such as well-posedness of appearing mathematical models (continuous and discrete), existence and uniqueness of solutions as well as convergence (globally? locally?) and convergence rate of proposed numerical methods. Due to the sheer scale of many problems as well as different magnitudes of scale appearing in many problems, parallelisation and domain decomposition are techniques to be looked into.

We present a domain decomposition Ansatz for partially saturated groundwater flow as well as a globally convergent and robust linearisation method to decouple and solve the discrete problem involved. The domain decomposition focuses on using different models on decomposed parts of the domain to accommodate different physical circumstances, such as vastly different permeabilities or porosities or coupling regions that are connected to the surface, to ones that are not.

We discuss rigorous analysis of the proposed scheme as well as numerical experiments.

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Modelling fractured porous media as coupled porous-medium and free-flow systems

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Fractured porous media are typically modelled as two different flow systems where two porous-medium models are coupled at the fracture-matrix interface. Usually, the flow in the fracture and in the matrix is described by the same model, which is Darcy's law. When the flow rate in the fracture is large enough, the Forchheimer extension of Darcy's law is applied in the fracture, while Darcy's law is used in the matrix. Recently, for modelling fractures and open channels, a Brinkman-Darcy model is proposed.

In this presentation, we consider fractures that act as channels, where most of the fluid is stored and transported, and model fractured porous media as coupled free-flow and porous-medium systems. The fractures are treated as the free-flow region described by the Stokes equations and the solid matrix represents the porous-medium system described by Darcy's law. The model formulation including appropriate coupling conditions at the fracture-matrix interface and efficient numerical methods based on adaptive time-step splitting schemes will be presented.

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Modelling root water uptake on the pore scale: Concepts to include the properties of the rhizosphere

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Transpiration accounts for approximately half of terrestrial precipitation yet recent and ongoing experimental research shows that root water uptake is not fully understood. The properties of the rhizosphere differ greatly from that of the bulk soil, an experimental finding that is mostly ignored in standard root water uptake models . Roots modify the soil in several ways. They exudate mucilage, a polymeric gel which retains large volume of water during drainage and turns hydrophobic after drying (Carminati, Vetterlein 2013). These properties are hard to include in an REV approach therefore in this work a pore- network model coupled to a root model on the continuum scale is used to implement these properties on the pore scale. The fully implicit pore network model is used to describe the rhizosphere whereas the bulk soil is discretized on the Darcy scale and is coupled to the pore network model as well. This means that in this work a system of a pore network model is used at the interface of root and soil which describes the processes at that interface better. A new concept is developed to include mucilage explicitly in the pore network model as a quasi solid phase which alters the geometry of the pores and throats. Being present as a extra phase, the mucilage is able to shrink and swell and retain the water during drying. The wettability change after drying can be described with the contact angle being a function of water saturation. The concept will be implemented in the open source simulator DuMux.

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Numerical investigation of initiation of sediment transport using Smoothed Particle Hydrodynamics

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Suspensions and their applications can be found in many fields of mechanical, civil and environmental engineering. One example for this is the mobilization of solid grains at the interface between a free flow domain and a porous domain, i.e. initiation of sediment transport. For this special kind of initiation of particle motion and sediment transport in general, various theoretical models exist to approximate critical values in the interfacial region. Most of these approaches base on two-domain formulations [1] or one-domain formulations [2]. We validated these theoretical models with 2D Direct Numerical Simulations in [3]. The results of these simulations showed that the theoretical models often underestimate the occurring velocities at the interface and therefore critical velocities to initialize the motion of single grains can be lower than predicted by the theoretical approaches. Moreover we found an increasing formation of vortexes with increasing heterogeneity at the interface. Thus our aim was to extend the numerical model to 3D applications to study the fluidization of a solid grain bed more realistically.

We present 3D Direct Numerical Simulations of a single-phase fluid with embedded solid particles to consider the flow behavior and fluid-solid interactions as in thin suspensions. Following what was presented by [4] we therefore present an implementation using the molecular dynamics particle code HOOMD-blue extended for the usage of Smoothed Particle Hydrodynamics (SPH) [5, 6]. Since both the fluid and the solid part can be discretized by particles, SPH as a particle method of Lagrangian character presents a good choice to model this particular non-linear problem. We first discuss the scaling behavior of our implementation by simulating known benchmarks on a cluster with 52 execute nodes each including 20 cores. Furthermore, we study the flow behaviour of suspensions using 3D Direct Numerical Simulations. Therefore, we implement numerical applications to model single and multiple spherical solid grains in a single-phase Newtonian fluid under different boundary conditions as for example gravity or shear flow. Afterwards the resulting particle velocities and shear stresses can be considered and compared to known analytical solutions. Different to what was shown in [4], we want to focus on the pore scale effects as for example the mobilization forces acting on a bed of solid grains as well as the transformation of flow behaviour dependent on the number of suspended particles.

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Pore scale velocimetry – application to mass transfer between fluid phases

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This project focusses on mass transfer between different fluid phases during multiphase flow in porous media. Due to its relevance for groundwater remediation, characterization of contaminated sites, oil & gas production, CO2 storage, and the use of natural tracers, the topic has been studied intensively. There are an abundance of models available that describe this process. Yet, none of these models are based on direct observations of the underlying processes at the pore scale (~ 1-100 µm). The goal of this project is to develop a continuum model for mass transfer on the cm scale based on observations of the 3D flow field during multiphase flow. A particle tracking random walk scheme, which runs on the observed flow field, will be used to classify areas of distinctive mass transfer. Based on this classification a continuum model for mass transfer will be developed. Pore-Scale Observations General defocusing particle tracking has been successfully applied to measure velocity fields in single phase flow in a measurement volume of 1510 x 1270 x 160 µm3 (Barnkob, et al., 2015). They dispersed fluorescent microparticles in a fluid that matches the refractive index of the solid. Images of the microfluidic device are magnified with a microscope and captured with a high-speed camera. The distance that a particle moves between two images reveals the local velocity. In this study, the method of (Barnkob, et al., 2015) will be extended to multiphase flow, where it is crucial to capture the interface between the fluid phases. A rectangular tube filled with sintered porous glass is used as the solid medium and two fluids are going to be co-injected into the medium. Pore Scale Simulations & Development of Continuum Scale model Mass transfer is simulated on the pore-scale by using a particle tracking scheme based on the approach of Pereira Nunes et al. (2016). Pereira Nunes et al. (2016) developed their model for the dissolution of carbonate rock by the injection of a weak acid. They calculate the single phase flow field by solving Navier Stokes equation. The advective-diffusive transport within this fluid is determined with a Lagrangian particle tracking approach. In this study the goal is to run the computational particle tracking scheme directly on the experimentally determined flow field. This allows for the determination of rates of mass transfer across the whole fluid-fluid interface. For specific flow conditions the total rate of mass transfer can be determined in a representative elementary volume. This is done by multiplying the rate of mass transfer with the respective interfacial area.

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Pore-scale mechanisms of water repellency in the rhizosphere

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Roots are known to exude a significant amount of organic compounds into the soil. One of these exudates called mucilage is released at the tip of roots during growth and known to turn water repellent when dry. A similar effect is observed for dry soil with critical content in organic matter. We investigated the natural distribution of mucilage of various concentrations in soil and its effect on the magnitude of water repellency employing the sessile drop method. Our results showed a distinct threshold-like behaviour when mucilage concentrations reached a critical level at which soil turned hydrophobic. This critical concentration decreased with increasing particle size. For repacked samples a moderate increase in contact angles with increasing concentration was observed. Our findings can be explained by a preferential distribution of mucilage in the contact region between soil particles. During drying water menisci recede and draw mucilage towards the inter-particle space where it is deposited. For low concentrations, this region is bypassed by water and the apparent contact angle is small. With increasing amounts of mucilage, the size of deposits expands into the open pore space, blocks water flow and results in a high contact angle. Additionally, this process was observed on rough particles, causing a shift in critical mucilage concentrations towards higher concentrations due to a more uniform distribution of mucilage across particle surfaces. Light microscopy images showed this process of preferential distribution and the additional effect of surface roughness.

This study shows the impact of non-uniform pore-scale distribution of organic matter (in this case mucilage) on soil water repellency and explains the criticality of this process.

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Scaling of Convective Velocities in Buoyancy-Driven Instabilities Of Miscible Interfaces

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Fingering instabilities of a miscible interface between two different fluids can develop due to buoyancy-driven Rayleigh--Taylor or double diffusive effects. Rayleigh--Taylor instabilities occur at the interface between a dense fluid above a less dense one in a gravitational field [1, 4] whereas double-diffusive instabilities arise due to the differential diffusion of components such as solutes and heat triggering the convective motion [2, 3]. These instabilities play a role in a plethora of natural processes and industrial applications such as transport of sediments and ground water, thermohaline convection in oceans, crystallisation in magmas, thin film flows and oil recovery, carbon sequestration in aquifers, to name a few. The respective roles of the instability mechanisms have been quantified experimentally, theoretically, and numerically during recent years. Here, we show that the driving force behind the convective growth of the related fingers, in particular, the mixing rate, can be explained using a generalised scaling law. Contrary to previous studies where the finger velocity was associated with the initial density difference between the two layers, and to the ratio of diffusion coefficients of the species involved, we show here that the density jump that arises after the initial time controls the growth of the instability, irrespective of the mechanism that generates it. A general scaling that governs the rate of advancement of the mixing front has been verified numerically by simulations of Darcy's law coupled to evolution equations for the concentrations of different solutes changing the density of the fluids. The scaling is further verified experimentally by a study of mixing between two different solutions in a Hele-Shaw cell. In this context, we unify both the Rayleigh--Taylor and double-diffusive instabilities by providing a general explanation that governs the dynamics of these instabilities.

Keywords: Rayleigh--Taylor Instability, Double-Diffusive Instability, Porous Media, Hele-Shaw Cells

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The Vapour-vapour Interphase Oberservation and Simulation of a Gas-Condensate/ Supercritical CO2 system

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Injectng supercritical CO2 into gas reservoir is a novel trial to improve condensate gas recovery and decrease the hydrocarbon liquid dropout. A good understanding of the effect of supercritical CO2 on the phase behavoir peroperties of these hydrocarbons is essential for accurately forecasting the displacing performance and storing process of the reservoirs with numerical simulators. This paper presented novel phase behavior experimental procedures and phase equilibrium evaluation methodology for gas-condensate phase system mixed with supercritical CO2 with high temperature. A unique phase behavior phenomena was also reported. The mass transfer time between two vapour phases was also measured. In order to interpret and identify condensate gas and supercritical CO2 interfacial phenomena, multiphase thermodynamic VVL equilibrium model considering interphase between condensate gas and supercritical CO2 was established. Finally, taken YKL condensate gas in Northwest China as example, the region where the conditions in terms of pressure, temperature and CO2 concentration can yield VVL equilibrium was found. Three phase hydrocarbon thermodynamic parameters with CO2 displacing YKL condensate gas were calculated with multiphase thermodynamic VVL equilibrium model, which were consistent with the PVT experiment data. The research results indicated that under certain condition, CO2 could be attractive option to successfully displace condensate gas and decrease CO2 emissions, which is a promising technology for reducing greenhouse gas emission and increasing ultimate gas recovery of condensate gas reservoir.

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Time scales of relaxation dynamics during hydraulic non-equilibrium in two-phase flow

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The relaxation dynamics towards a stable equilibrium after a change in phase saturation in porous media is governed by fluid reconfiguration at the pore scale. Little is known whether a true equilibrium is ever reached and which microscopic processes govern the time scales of relaxation. Here we apply fast synchrotron-based X-ray tomography to measure the relaxation dynamics of fluid interfaces in a glass bead pack after fast drainage of the sample. The relaxation of interfaces triggers internal redistribution of fluids, reduces the surface energy stored in the fluid interfaces and relaxes the contact angle towards the equilibrium value while the fluid topology remains unchanged. This equilibration of dynamic capillary pressures occurs in two stages: (i) a quick relaxation within seconds in which most of the pressure drop that built up during drainage is dissipated and (ii) a slow relaxation with characteristic time scales of 1-4h that is well described by the Washburn equation for capillary rise in porous media. The slow relaxation implies that true equilibrium is hardly ever attained in practice when conducting two-phase experiments, so that dynamic effects may falsely be identified as hysteresis.

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Upscaling of coupled free-flow and porous-media-flow processes with droplets

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The objective of this poster is the development and testing of an REV-scale coupling concept that accounts for drop dynamics at the interface between free and porous-medium flow. In particular, drop formation, growth and detachment on a hydrophobic interface is described. The interface stores the mass and energy of the drops without resolving them. Besides the drop coupling, the direct exchange between free-flow and porous medium region next to the drop is also part of the coupling concept. The temporal evolution of the drop volume is an outcome of the model, whereas the number of drops that can form on the interface is defined a priori. The simulations for a higher number of drops suggest that the interface conditions dominate the system. On a specific example the performance of the new coupling concept will be discussed.

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Using a pore-network model to couple mass, momentum and energy at the interface between free flow and porous media flow

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Coupled systems of free flow and flow in porous media appear in a wide range of industrial and environmental processes. A well-established modeling approach for these kinds of problems comprises the partitioning of the system into two separate domains and applying two different types of equations on each domain, e.g. the (Navier-) Stokes equations for the region free flow and Darcy's law for the porous medium. However, this approach requires the formulation of explicit coupling conditions at the interface between the two sub-domains which can be a challenging task. Commonly, an interface of infinitely small thickness devoid of thermodynamic properties ensures the continuity of fluxes as well as thermodynamic equilibrium (e.g. Mosthaf et al., 2011). While this approach is capable of resolving interface-related processes such evaporation only in an averaged sense, the potential spatial non-uniformity, e.g. due to capillary effects, of these processes may have a decisive influence on the global system behavior (Shahraeeni et al., 2012).

One further issue of the above-mentioned two-domain approach is the proper description of the tangential momentum transfer between the two flow regimes. The widely used Beavers-Joseph-Saffman condition (Saffman, 1971) was developed for a rather simple flow configuration and its applicability for multi-phase systems with a flow direction not entirely parallel to the interface remains questionable.

We propose a new kind of approach where the interface region between free flow and porous medium is described discretely using a dynamic pore-network model. This results in a model comprising three domains: the porous medium described by Darcy's or Forchheimer's law, the interface region represented by the pore-network model (Joekar-Niasar et al., 2010) and the region of free flow where the (Navier-) Stokes equations are applied. If necessary, mortar elements can be used to couple these three domains (Mehmani and Balhoff, 2014).

As a first step, single-phase flow of water through a micromodel is considered where experimental data are available. Following this, the model will be extended in such a way that it can describe compositional, non-isothermal two-phase flow which is a prerequisite for modeling evaporation processes.

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Incorporating freezing/thawing process into a coupled water and heat model

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Representing Freezing/thawing process is of great importance in cold region climate studies. However, it is full of challenges as both soil water and heat are necessary to be accurately captured. In this study, we aim to develop a numerical method based on Simultaneously Transfer of Energy, Mass and Momentum in Unsaturated Soil (STEMMUS) model to: i) solve the coupled soil water and heat transfer with water phase change; ii) investigate the interaction effect of uncertainty in soil properties (porosity, soil texture) and frozen process on the simulated results. A new state variable, soil ice content, was introduced and estimated by the combination of soil water characteristic curve (SWC) and soil freezing curve (SFC). The latent heat for water phase change when soil was frozen was considered in the heat transport module. Results showed that the proposed model was capable of reproducing the movement of soil moisture and heat flow in frozen soil. Further examination of the influence of the uncertainty in soil properties highlighted the important role of soil properties in simulating water and heat transfer during soil is freezing/thawing.

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Pore condensation in capillary porous media during superheated steam drying: influence of heating mode on phase distribution and drying kinetics

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In superheated steam drying (SSD), the volatile liquids are removed from natural or finished solid materials by using superheated steam as the drying agent. Compared to hot air drying, this drying technique has several specific advantages such as higher drying capability due to the high thermal conductivity of vapor, and a better product quality since the oxygen content is much lower [1]. Although widely used in food, medical, and other industries where drying plays a crucial role, transport phenomena in porous media exposed to superheated steam have been mathematically described merely by continuum-scale models [2]. In these models, for a given porous medium, properties such as the wettability, pore shape, pore size distribution, and pore structure are lumped together in several effective transport and equilibrium parameters. These parameters have to be determined by experiments, which is time-consuming since they depend on the liquid saturation. The estimation of these parameters by advanced theoretical models is still to come [3]. In this work, a non-isothermal two-dimensional pore network model which incorporates the relevant transport processes is developed to simulate the SSD of capillary porous media. In this model, the complex void space of the porous medium is approximated by a network of spherical pores interconnected by cylindrical throats. The liquid transport in the porous medium is driven by capillary action, whereas the vapor transport occurs due to convection. Based on the assumption of local thermal equilibrium, the discrete dynamic energy balance equation at each pore is solved to obtain the liquid distribution and the temperature field in the medium. Due to the non-uniform distribution of temperature, condensation occurs in regions where the temperature is below the saturation temperature of vapor; whereas evaporation occurs in regions where it is above. To fully treat the pore condensation, a set of liquid invasion rules are introduced in this model. Simulations are carried out for two types of heating modes (see Fig. 1): (i) convective heating at the top surface and (ii) simultaneous convective and conductive heating at the top and bottom surfaces. These specific boundary conditions for heat transfer are adopted from practices. Thus, a porous sample can be heated either by convective only or with the assistance of microwave or contact heating to accelerate the drying process. Figure 2 shows the thermal and hydrodynamic behavior in a pore network with these heating modes.

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Sand fluidisation and its role for diurnal fluctuations of water levels in streams and rivers

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Mechanisms responsible for observed in field conditions diurnal fluctuations of water levels in streams or rives and groundwater levels are poorly recognized (Gribovszki et al. 2010, Marciniak and Szczucinska 2014). Among phenomena which may cause the fluctuations are evapotranspiration, temperature dependence of transport properties (viscosity and permeability), precipitation or freezing-thawing processes, human activity. In some cases however at bottoms of shallow waters a fluidisation of sand is observed and it is hypothesized that this process may play some role in diurnal water level fluctuations. This work reports results of experiments in fluidised column with different types of sand. The dependence of discharge velocity on hydraulic gradient for increasing and then decreasing hydraulic gradient is observed. Critical hydraulic gradients for which the fluidisation sets in are determined and compared with predictions of the model based on two-phase continuum theory under condition of vanishing effective stress (Vardoulakis, 2004). The results of laboratory studies are taken into account in discussion of factors which determine diurnal water level fluctuations. Signal analysis is used to determine peculiarities of fluctuations, particularly for rainfall periods. Then, even a slightincrease of hydraulic gradient in groundwater is possible, which may result in fluidisation.

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Thermal diffusion of water vapour in porous materials: truth or myth ?

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Moisture often plays a crucial role in the durability and sustainability of built structures, as well as in the health and comfort of building occupants. A reliable evaluation of moisture transport in built structures, and thus in porous materials, is hence essential. Such reliable evaluation requires the correct description of the moisture flow phenomena and their related transport potentials. In that respect, thermal diffusion of water vapour – diffusion of water vapour in response to gradients in temperature – currently stands out.

Various studies in literature conclude that vapour pressure is the only significant transport potential for diffusion, and that thermal diffusion of water vapour is thus negligible; other results imply that temperature gradients do however similarly result in notable diffusion. While vapour diffusion is surpassed in magnitude by capillary liquid or advective vapour transport, it does form a noteworthy moisture transfer mechanism, crucial in evaluating material drying, interstitial condensation, moisture buffering, ... The current contradictory findings on thermal water vapour diffusion thus need to be investigated, in order to come to a more convergent conclusion on its (in-)significance.

This paper will reconcile the contradictory results on thermal diffusion. Introductorily, the thermodynamic foundations for water vapour diffusion in air will be concisely reiterated, providing a general background for the paper. The second section will investigate the studies confirming vapour pressure as sole significant transport potential for diffusion. In the main section of the paper, the analyses supporting thermal diffusion will be critically examined, and shown to be generally flawed. A corrected reinterpretation finally permits arriving at a convergent conclusion on the insignificance of thermal diffusion of water vapour in porous materials.

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Comparative Study on Capillary Trapping using Representative Microstructures with Smooth and Rough Pore-Solid-Interfaces

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We performed imbibition experiments in the range of capillary numbers (Ca) from 10^−6 to 5×10^−5 using 2D-micromodels [1-3]. We used a new method to generate representative micromodels (80 x 80 mm, about 10000 pores). First, the the 3D-microstructure was characterized by the 4 Minkowski functionals. Based on this the 2D-microstructure were produced by a global optimization algorithm (Simulated annealing) under the constraint of an equal Euler characteristic. Therefore, both the 3D- and the 2D-microstructure exhibit the same connectivity. We compared capillary trapping (i) in Silicon (Si)-microstructures (smooth pore-solid interface) and (ii) in Glass-ceramics-microstructures (rough pore-solid interface = surface). Both micromodels possess the same pore structure and the same connectivity. For the first time we proof experimentally that microstructures with rough surfaces show a different fluid-fluid displacement and trapping behavior. Whereas Si-microstructures show a compact front-displacement for the imbibition process (e.g. water displaces gas) and by-pass trapping, the fluid-fluid displacement process in Glass-ceramics-microstructures is characterized by precursor-thin film flow and snap-off trapping. (i) In Si-micromodels no visible precursor thin-film flow and no trapping in front of the advancing bulk water phase were observed. Hence, the trapping process is by-pass trapping. The multiphase-flow dynamics of the by-pass trapping process is piston-like, and no core-annular flow accompanied with capillary instability was observed. The whole trapping occurs within a transition zone as discussed by Wilkinson [4] given by the width of the rough interface that is approximately 4–5 mm. (ii) In Glass-ceramics-microstructures the dynamics of precursor thin-film flow and its importance for capillary trapping was studied. The experimental data for thin-film flow advancement show a square-root time dependence. Based on the experimental data, we conducted inverse modeling to investigate the influence of surface roughness on the dynamic contact angle of precursor thin-film flow. Our experimental results show that trapped gas saturation decreases logarithmically with an increasing capillary number. Cluster analysis shows that the morphology and number of trapped clusters change with capillary number. We found that our experimental results agree with theoretical results of percolation theory for Ca = 10^−6: (i) a universal power-like cluster size distribution, (ii) the linear surface–volume relationship of trapped clusters, and (iii) the existence of the cutoff correlation length for the maximal cluster height. The good agreement is a strong argument that the experimental cluster size distribution is caused by a percolation-like trapping process (ordinary percolation).

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On the evolution of interfaces and phase connectivity during viscous-dominated primary drainage in 2D porous media

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We perform pore-scale resolved direct numerical simulations of immiscible two-phase flow in porous media to analyze the mechanisms by means of which discrete fluid-fluid interfaces evolve. While pore-scale imaging methods, e.g. fast X-ray tomography methods, to study the distribution and evolution of fluid-fluid interfaces for capillary-dominated flow become increasingly mature [1,2], their applicability to viscous-dominated flow is limited by temporal resolution. We consider hydrodynamic direct numerical simulations (DNS) a suitable complementary approach to study viscous-dominated two-phase flow. Using a Smoothed-Particle Hydrodynamics model [3], we present DNS of primary drainage in partially wettable 2D porous media of particulate microstructure at large capillary numbers.

During viscous fingering, pore-scale flow fields are reminiscent of Bretherton annular flow, i.e. the less viscous phase percolates through the core of a pore-throat forming a hydrodynamic wetting film. Even in simple microstructures, wetting films are shown to have major impact on the evolution of fluid-fluid interfacial area and shown to give rise to non-negligible interfacial viscous coupling. Although macroscopically appearing flat, saturation fronts during stable displacement extend over the length of the capillary dispersion zone. While far from the dispersion zone fluid permeation obeys Darcy's law, the interplay of viscous and capillary forces is shown to render fluid flow within the capillary dispersion zone complex.

Recently, Schlüter et. al. (2016) demonstrated the fundamental role of fluid topology in permanent hysteresis effects during drainage and imbibition. A topological analysis of wetting phase connectivity during primary drainage is discussed as to emphasize on topological implications of 2D simulations. We critically discuss the topological constraints of 2D simulations by computing the Euler characteristic (χ) as well as the Betti Numbers of the wetting phase during viscous fingering and stable displacement. For viscous fingering, we emphasize on the isolation of wetting films and the resulting increase in χ which is likely not to occur in 3D systems. On the hand, for stable displacement, χ is shown to increase linearly with saturation which applies to compact displacement patterns in 3D systems as well [2].

Finally, we discuss future applications of SPH to model two-phase flow in 3d porous media using image-based data.

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Pore scale displacement mechanisms as a source of hysteresis for two-phase flow in porous media

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The macroscopic description of the hysteretic behavior of two-phase flow in porous media remains a challenge. It is not obvious how to represent the underlying pore scale processes at the Darcy-scale in a consistent way. Darcy-scale thermodynamic models do not completely eliminate hysteresis and our findings indicate that the shape of displacement fronts is an additional source of hysteresis that has not been considered before. This is a shortcoming because effective process behavior such as trapping efficiency of CO2 or oil production during water flooding are directly linked to pore scale displacement mechanisms with very different front shape such as capillary fingering, flat frontal displacement or cluster growth. Here we introduce fluid topology, expressed by the Euler characteristic of the non-wetting phase, as a shape measure of displacement fronts. Using two high-quality data sets obtained by fast X-ray tomography we show that Euler characteristic is hysteretic between drainage and imbibition and characteristic for the underlying displacement pattern. In a more physical sense the Euler characteristic can be interpreted as a parameter describing local fluid connectedness. It may provide the closing link between a topological characterization and macroscopic formulations of two-phase immiscible displacement in porous rock. Since fast X-ray tomography is currently becoming a mature technique, we expect a significant growth in high quality datasets of real time fluid displacement processes in the future. The novel measures of fluid topology presented here have the potential to become standard metrics needed to fully explore them.

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The missing link between the pore network topology and the residual oil saturation

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Classical macroscopic properties, describing an immiscible two-phase flow in porous media, fail to fully account for the complexity of the displacement mechanisms occurring at pore-scale. Consequently, properties such as the residual non-wetting phase saturation (Snwr) remain tricky to assess. Several studies have attempted to define a correlation between the residual trapped phase and the different parameters driving the imbibition process [1]. While it is acknowledged that there is a generally decreasing trend of residual saturation with increasing porosity the relationship between residual saturation and topological properties is not yet resolved [2]. Yet two main local trapping mechanisms have been observed experimentally [3-4]: the snap-off induced by the collapse of the wetting phase in the pore throat and the by-pass described by the pore doublet model [5]. In this work, we have considered the link between local and global topological properties of pore network and the resulting distribution of residual saturation. X-ray tomography and advanced porous network segmentation algorithms [6] have been used to investigate the micro-structure of porous media and the distribution of the non-wetting fluid trapped at the end of an immiscible sweeping. Experiments have been conducted on two clay-free water-wet homogenous sandstone (Bentheimer and Clashach). Micro-plugs with typical dimensions of 20mm in length and 10mm in diameter were imaged at dry condition and at residual oil saturation after a spontaneous imbibition. Then pore-scale geometrical properties of the porous media were computed as well as the distribution and the configuration of the oil ganglia trapped in the porous media. The results show that the two rock-types exhibit similar pore network local structural properties, namely pore and throat radius, coordination number and aspect ratio distribution. However the resulting Snwr and the ganglia size distribution are different. As a consequence no straightforward dependencies of the ganglia size distribution neither the Snwr to these statistical parameter is observed. The difference between the two rock-types is clearly observed by analysing the pore neighbouring environment. To access this topological property we have computed a semi-variogram that reports pore size variance of neighbors of order h (for two adjacent pores h=1) normalized by the global variance of the pore size distribution (cf. Fig 1). The comparison of the Bentheimer and Clashach semi-variogram (cf. Fig 1) shows that the Bentheimer rock-type has a pore layout twice more contrasted (i.e difference between pore size of close neighbors is more important) than the Clashach rock-type. Linking this property to the by-pass mechanism can then explain the differences observed on the ganglia size distribution (cf. Fig 2). Indeed the by-pass mechanism is governed by the contrast between neighbor pores, as the more the contrast the smaller the trapped ganglia are.

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A Cahn-Hilliard Approach to Thermodiffusion in Porous Media

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For a given physical system, we observe a cross effect [1], when the flux of an extensive quantity (for instance, heat or mass) can be related not only to the gradient of the state variable that is directly linked to it (i.e., temperature and chemical potential, respectively), but also to the gradients of the other state variables of the model. Thus, if the Onsager-Casimir relations are exploited, the flux of the considered extensive quantity depends linearly on the gradients of all the other state variables [1].

In this contribution, the cross-effect giving rise to thermodiffusion, also known as Soret effect, will be discussed in the framework of density and temperature driven flows in porous media. In a mixture exposed to a non-uniform thermal field, this phenomenon occurs when the thermal gradient is capable of inducing the mass flux of the species of the mixture.

In a thermogravitational cell, due to the presence of concurrent buoyancy and thermal forces, an initially uniform mixture separates. We present numerical results of such experiment, retrieved by means of the standard thermodiffusion model, and compare them with experimental evidences, and previous results available in the literature [2,3,4]. Finally, we discuss the practical and theoretical consequences of choosing, in the framework described so far, a Helmholtz free energy density of the Cahn-Hilliard type [5].

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Dynamic tracking flood front of the reservoirs using magnetic fluid

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In the process of reservoir development, the equilibrium displacement is implemented by adjust the development plan according of the production pressure and producing liquid. But there is still no technique to realize the dynamic detection of the water-oil displacement. In this paper, we model the secondary magnetic field which is generated by the magnetic fluid in the reservoir and build the relationship between the secondary magnetic field and the position of the magnetic-fluid. Finally, we track the flood frond according that the magnetic field change over time in the waterflood. Magnetic fluid as a kind of new materials has been widely used in the generator, biomedicine and other fields. Without the super paramagnetic magnetic, the performance of the magnetic fluid is as same as the general fluid. While when applied in the magnetic field, the magnetic fluid will be magnetized and then generate a secondary magnetic field at the same time. In the process of reservoir development, the transmitter in one well broadcasts the external magnetic field and the multiple receivers detect the magnetic strength in the other wells or on the surface. When no magnetic liquid injected, the receivers detect the magnetic strength B0 which is the external magnetic field, while when magnetic fluid injected, the receives detect the magnetic strength B is the sum of external magnetic field's B0 and secondary magnetic field's B'. As the magnetic fluid moves in the reservoir, the detecting value from the receivers are varying with the magnetic fluid position. There is a mathematical relationship between the variation of the magnetic strength and the position of the magnetic fluid $\Delta B=f(x-x0,y-y0,z-z0)$, thus we would realize the dynamic tracking the flood front of the reservoir.

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Modeling Moisture Transport Through Partially Saturated Porous Media at the Pore Scale Using Chemical Potential

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Here we use chemical potential to model vapour transport through partially saturated porous media at the pore scale with variable cross-sectional area, demonstrating the simplicity of the model formulated in terms of chemical potential and the clarity it provides in explaining the enhancement factor (often used in hydrology) and other physical observations without explicitly modelling e.g. the surface curvature and tension. The numerical results are favourably compared with experiments, and the movement of the liquid bridge and the lack of steady state (assumed to exist by the experimentalist and other researchers who have modelled this problem) are explained.

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Moisture and water transport including mass exchange in swelling cellulose fiber materials

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Situations where paperboard is exposed to unfavourable environments are many, e.g. in the manufacturing of paperboard based packaging material one possibility to sterilize the material is by using water-peroxide baths. Another situation is the sterilization of filled and sealed packages where the paperboard material is exposed to liquid water and elevated temperatures. Since the cellulose fibers in the paperboard has a natural high affinity towards water, a remedy is to modify the surfaces of the fibers such that it becomes hydrophobic in order to endure under these conditions. This modification of the fibers will change some of the possible water-fiber interactions. The uptake of water in cellulose fiber will cause swelling of the fibers as well as change of the mechanical properties of the paperboard. It is therefore of importance to understand the transport of moisture through the material to be able to design good packaging materials as well as controlling the transport processes to ensure package integrity. In this work we use hybrid mixture theory to derive a thermodynamically consistent model that can predict edge wicking and moisture transport properties of paperboard. The paperboard is modelled as a three-phase material where the phases are solid (fibers), liquid water and air. The fiber is further separated into a dry fiber and fiber-wall water and the air is viewed as a miscible mixture of dry air and water vapor. The phase-interfaces are accounted for in the formulation to account for a wider range of phenomena. This enable us to model several different modes of water transport including in-fiber diffusion, bulk water transport via capillary forces and vapor diffusion. Transfer of water between the different thermodynamic states are also addressed in a non-equilibrium fashion [1]. Macro-scale constitutive relations are derived from the dissipation inequality [2], where it follows that the chemical potential of the different water states are the driving force for mass transfer as well as diffusion [3]. The swelling of the fiber phase is postulated to depend on the bound water content and experimental data from hygro-expansion are used to find the material parameters. The model is used to simulate the material behaviour and response when subjected to liquid water and/or water vapor and elevated pressures as well as mechanical loads with the aim to understand the relative importance of the different mechanisms.

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Numerical efficiency of different moisture potentials for simulation of miosture transfer in building materials

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Heat and moisture play a crucial role in the durability and sustainability of built structures and in the health and comfort of building occupants. A reliable hygrothermal analysis of built structures is thus often essential. In this, the use of numerical simulation models for heat and moisture transfer in materials and components are becoming progressively more common. Several hygrothermal simulation models are available to that purpose, each with specific modelling preferences and simulation capacities. One of the fundamental differences between models is the potential used to describe the moisture storage and transport: moisture content, vapour content, capillary pressure, log of capillary pressure are a few examples. Complementary to physical reasons, numerical arguments are often suggested: use of a certain potential is favoured for its 'numerical efficiency', 'reducing non-linearity', ... Solid foundations for those arguments are however lacking, and a supported choice is thus difficult to make.

In an introductory paragraph, physical arguments for the selection of certain storage and transport potentials for moisture are summarised, and the reference simulations for the assessment of their numerical efficiency are formulated. These reference simulations involve ad- & desorption, isothermal drying and free water uptake. In the core section of the paper, these reference simulations are performed based on different potentials, and their impact on numerical efficiency is investigated. The latter is quantified by means of necessary number of time steps and iterations to complete simulations, and by means of necessary number of discretisation nodes to maintain accurate solutions, in comparison to a reference solution. Such evaluation allows deciding which potential is most efficient for numerical models, which will in turn decrease the computational expense, and hence grow the applicability of hygrothermal simulations.

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Studies of the vapor-diffusion enhancement in concrete using experiments and a two-phase moisture transport model

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The dependency of moisture transport coefficients on the saturation degree for ten different cement binders is investigated experimentally and modeled using a two-phase moisture transport model proposed by Johannesson and Nyman [1], where the saturation degree and the relative humidity (RH) are the main unknowns. The relation between the saturation degree and the diffusion of water vapor and liquid water is central in the model. These relations cannot be measured individually but the overall effect can be measured using different techniques. Four different experimental setups where carried out to capture the effect of saturation degree on moisture transport in concrete. The experiments used are (i) dynamic vapor sorption measurements on paste samples (moisture fixation), to provide the sorption isotherms for the ten different cement binders in use, (ii) 1D drying experiment on paste samples with fixed outer drying climate (33% RH), (iii) 1D cup measurements where samples are exposed to two different fixed RH conditions on both ends (two set of samples with 75-85%RH and 85-95%RH, and (iv) capillary suction experiments where samples are first dried to a known RH and then put in contact with water, to study the effect of capillary suction. The results from experiment (ii), (iii) and (iv) where used to back calculate the effective diffusion coefficient curves for the water vapor and liquid water. Findings from Addassi et al. [2] motivated the choice of functions in which the effective vapor diffusion increases with increased water saturation due to the enhancement factor, that is, the travel path for the vapor assumed shortened by increased saturation. It is considered that the effect of liquid water diffusion can to some extend be neglected at RH intervals below about 95%RH but is very dominant at 100%RH due to the capillary suction effect. It was possible to find effective diffusion curves for the vapor and liquid phase resulting in a good match between the experimental data and the numerical model.

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Characterization of pore deformation and damage using x-ray scattering methods

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Since the discovery of mesoporous materials small-angle x-ray scattering (SAXS) has been considered a valuable tool for their characterization, particularly for addressing surface area, porosity, size, shape and arrangement of the pores. In last years, this method gained also considerable attention for the investigation of first ordered phase transitions in nanopores. Complementary to SAXS, wide angle x-ray scattering analyses (WAXS) represent a valuable tool to correlate the changes of the pore structure with the crystallization of the guest species. Despite the widespread technological implications (e.g. conservation of construction materials, energy storage), the phase change behavior of salts in nanopores and its effect on the confining body is to a large extent still unknown. With this respect, in the present paper we show a systematic characterization of salt conversion in ordered porous hosts depending on the pore geometry parameters, such as pore size and shape. Using a combination of SAXS and WAXS methods we can address the structural changes of both host and guest material in direct and comprehensive fashion.

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Coupled THM constitutive model for porous materials under frost action: Application to frost heave simulation

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Soil freezing process may sometimes be accompanied by ice segregation and could result in frost heave phenomenon. Frost heave causes many engineering problems like pavement cracking, foundation damages and pipeline fracturing. Frost heaving is the result of water migration to the freezing front due to the so-called cryogenic suction. Cryogenic suction appears by the thermodynamic equilibrium between ice and liquid water phases. Numerical simulation of these phenomena requires a coupled thermo-hydro-mechanical (THM) model including mass, energy and momentum balance equations (e.g. Thomas et al., 2009; Nishimura et al., 2009). In addition to the global governing equations, a mechanical constitutive model which is able to provide the possibility of plastic volumetric deformation due to temperature variation and with respect to the hydraulic condition, is also required (e.g. Ghoreishian Amiri et al, 2015). This paper aims to introduce a coupled THM constitutive model and examine its applicability for simulating such a phenomenon. From the point of view of material science, saturated frozen soil is a kind of composite material composed of solid grains, ice and unfrozen water. Existence of ice and its interaction with solid grains and unfrozen water, make the mechanical behavior of frozen soil very different from the common soils. The ice content, temperature, confining pressure and hydraulic condition can be mentioned as the most important factors influencing the mechanical behavior of such a material. In this paper, a two stress-state variable model with a kind of effective stress and cryogenic suction is considered to reflect all of the above mentioned effects. The effective stress of the model is defined as the combined stress of soil grains and ice and it is responsible for considering the deformation due to variation of mechanical loads. The cryogenic suction which is defined as a function of temperature, is responsible for considering the temperature induced deformation (e.g. frost heave). In addition, unfrozen water saturation can reflect the local hydraulic condition of the composite. Thus, in the proposed model, an unfrozen water saturation dependent yield and potential functions are designed to consider the effect of the hydraulic condition. The proposed model is consistent with the micromechanical description of the behavior due to variation of ice content and temperature (Wettlaufer and Worster, 2006); i.e. curvature-induced premelting and interfacial premelting mechanisms (figure 1). The former is the result of surface tension and acts very similar to the capillary suction by bonding the grains together . Whereas the latter is the result of disjoining pressure (as a repelling force between ice and solid grains) and tends to widen the gap by sucking in more water. The proposed model is implemented in PLAXIS and its application is illustrated by simulating a frost heave deformation due to a chilled pipeline buried in unfrozen ground.

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Evaluating the influence of temperature on the hydraulic properties of unsaturated soils: a new soil column apparatus for transient-state tests

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Thermo-active piles has been recently proposed for slope stabilisation. Through the heating of the piles, the increase of the temperature of the surrounding soil would induce a decrease in soil matric suction, hence an increase in the soil shear strength for contributing to the slope stability, in addition to the mechanical pile reinforcement. The effectiveness of such a stabilizing system is strongly related to the thermo-hydraulic behaviour of the soil surrounding the piles. The hydraulic behaviour of unsaturated soils that govern the interdependence of soil water content, hydraulic conductivity and suction are soil water retention curve (SWRC) and soil hydraulic conductivity function (SHCF). Although there are various methods developed for the measurement of the two soil hydraulic properties, only a few of them can measure these two properties simultaneously using the same soil sample non-isothermally. In this presentation, a new soil column apparatus that can measure the influence of temperature on the hydraulic properties of unsaturated soils using a transient state method will be introduced. The proposed device (Figure 1) allows the direct measurements of the SWRC and the SHCF by means of the instantaneous profile method (IPM). By controlling the temperature of the soil column, the device allows to control different temperatures when measuring instantaneous profiles of soil water content and matric suction, based on which the SWRC and SHCF can be determined on the basis of mass continuity and Darcy's law. In the first part of the presentation, the detailed setup and the working principle of the soil column apparatus and of its working principle will be presented. The second part will report the measured results of pluviated sand and compacted silt at 20 ˚C and 50 ˚C. Any effects of temperature on both the SWRC and the SHCF of the two soil types will be discussed.

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Hydraulic properties of siliciclastic geothermal reservoir rocks under triaxial stress conditions, a multidisciplinary approach.

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Cretaceous Sandstone bodies in the subsurface of western Netherlands are already used for heating some of the greenhouses in that area. The reservoirs used are typically at an initial temperature of 75 ˚C. For higher temperature applications (i.e., above 100 ˚C) deeper reservoirs are required. However, deeper reservoirs are subjected to higher effective pressures due to more overburden, which can lead to more compacted rocks, and thereby reduced permeability. We assess the effects of effective pressure on Triassic Buntsandstein, a formation targeted to act as a deep geothermal reservoir in the western Netherlands. Rock samples are acquired from laterally equivalent quarries and prepared for permeability measurements within a tri-axial apparatus. To determine anisotropy, cores are drilled both perpendicular and parallel to bedding. Experiments are conducted by maintaining hydrostatic confining pressure, stepwise increasing up to 425 bar, and a pore pressure of 25 bar, conditions of roughly 2 km depth. At each step the permeability is assessed by imposing a number of constant flow rates and continuous measurement of the pore pressure difference. Throughout the experiment the sample strain is measured in radial and axial directions, such that elastic constants can be determined, and micromechanical mechanisms may be observed. Based on the collected data, the validity of the available exponential models for describing the permeability-porosity-stress relationship is assessed and the model parameters with the best fitting characteristic is chosen for the selected formation. The established relationship is then used as an input for field scale simulation of cold fluid circulation in Buntsandstein formation in a numerical framework. The Finite Element Method is used to evaluate the reservoir behavior during injection/production of the cold/hot fluid in a fully coupled poro-thermo-elastic environment. The results of this study show a promising capacity of heat extraction from the Buntsandstein formation as a geothermal reservoir.

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Long-Term Ground Response For Borehole Heat Exchangers In Clay

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The use of ground source heat pumps to transfer heat to and from the ground via borehole heat exchangers is among the most energy efficient techniques for space heating and cooling. Designs for seasonal heat exchange systems are becoming increasingly popular in urban environments to reduce energy costs and contribute in decreasing carbon emissions. Broader applications require more careful evaluation of hydro-mechanical behavior of soil to understand the long-term ground response to seasonal cycles of heating and cooling and the impacts on adjacent structures. The goal of this research is to develop reliable methods for studying the coupled thermo-hydro-mechanical (THM) response of clay to long-term seasonal heating and cooling induced by vertical heat exchanger arrays in clay. The research investigates and implements a new class of constitutive models based on the work by Zhang and Cheng (2013). The proposed Tsinghua Thermosoil (TTS) model is capable of simulating the cyclic thermo-mechanical response more realistically than other available constitutive models and can describe the accumulation of volumetric strain due to cyclic heating and cooling. Irreversible deformations in the TTS model are simulated through the conversion of bound to free water, a process that has been studied via laboratory measurements of specific gravity variations with temperature for three clays of differing mineralogy. The TTS model is integrated within a finite difference framework to solve coupled THM problems in the axisymmetric space. The FD simulator is applied to a prototype project that uses an array of borehole heat exchangers for seasonal heating and cooling. The ground conditions represent typical stress history profiles found in Geneva, Switzerland. The TTS model has been calibrated for Geneva clay using recently published cyclic thermal tests (Di Donna and Laloui, 2015). The results show that significant settlements can be induced due to their long-term operation (i.e., over periods from 10 – 50 years), especially within normally consolidated clay. The study provides a systematic framework for analyzing the long-term THM response of clay to seasonal heating and cooling. These analyses highlight the need to incorporate geotechnical characterization in the design of large borehole heat exchanger arrays to ensure their reliable long-term performance and to minimize adverse effects on adjacent structures.

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Micro-Scale Model of Thermomechanics in Solidifying Saturated Porous Media

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Among industrial or environmental issues related to cold regions all over the world, one can still find some phenomena that are not completely investigated and might have relevant impacts on the issues. Volumetric changes of a wet medium presented in pores of a porous material subjected to freezing/thawing conditions can be included among the phenomena ([1]). In order to enhance the knowledge on freezing problems, this contribution deals with this phenomenon.

As we believe that investigation of the phenomenon at the micro-scale is needed to understand properly its dynamics, we have developed a micro-scale model describing mechanical, thermal, and phase change processes within a small sample of a porous medium. The problem of phase change is described in the Lagrangian framework by means of the heat, Navier, and phase-field equations. A coupling of multi-physics and multi-phase is introduced. The model provides spatial-temporal dependencies of the all coupled quantities, the resultant forces exerted on grain surfaces by the freezing action, as well as the time courses of the mean values of the quantities. Several computational results are presented. The model outputs are believed to improve the phenomena description in the macro-scale models ([2]) through upscaling.

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Numerical simulation of thermo-hydro-mechanical process during hydraulic fracturing treatments

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The effect of thermo-hydro-mechanical process on hydraulic fracture propagation is of much interest in geothermal and petroleum related geomechanics problems due to its critical role in the development of enhanced geothemal system and tight oil/gas fields [1]. Generally, this process involves coupled rock deformation, fluid flow, heat diffusion, fracture extension and thermo-poroelastic effects in the fluid-saturated porous rock [2]. In this study, a fully coupled thermo-hydro-mechanical model is proposed to simulate hydraulic fracture propagation. The fluid-heat flow is solved using finite volume method, and rock deformation is solved by finite element method. They are solved simultaneously to obtain the fracture profile, the distribution of fluid pressure and temperature in the model. The numerical results are then compared with that of the model which does not consider the thermal coupling effects. The results show that temperature field can have significant influence on the fracture propagation behavior, especially for that with high temperature contrast between fracturing fluid and rock. Besides, the model is used to investigate the simultaneous propagation of multiple hydraulic fractures. Results show that the geometry of multiple fractures is strongly affected by the stress shadow effect and thermal stress. When it comes to unconventional reservoirs, the thermal stress may induce many secondary fractures perpendicular to main hydraulic fractures, which could effectively improve production well performance. Finally, the model is used to investigate the formation and propagation of secondary fractures.

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The design of a new field-scale energy pile experiment

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Thermo-active structures, where heat exchangers are embedded into structural elements, are becoming increasingly well recognised as a method of renewable generation or storage of heat. Heat exchangers are embedded into concrete structures to reduce the initial cost of installation and to take advantage of the positioning within or close to bulk materials which can act as heat sources/sinks. A direct consequence is thermal expansion/contraction, leading to thermal stresses, which should be fully understood to enable good design. In this work a new field test involving an energy pile is described. The objective is to better understand the thermo-mechanical behaviour of the soil and pile system, including changes in the shear resistance, the bearing capacity and the impact of long-term thermal cycles. Figure 1 outlines the main heat flows and mechanical changes anticipated. Details of the experimental programme, the mechanical design, the thermal behaviour and the sensoring are discussed.

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Thermal Performance of an Aquifer while Charging-Discharging Thermal Energy

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With the progress of human civilization, demand for energy and power is rising rapidly. As the fossil fuel reserve on the planet is reducing and will be exhausted in not so far future, use of renewable energy and energy conservation is becoming utmost important. Storing excess or waste thermal energy in aquifers is a favorable option in terms of feasibility and economy which is being used for last few decades. Storing seasonal thermal energy or waste heat from other sources in groundwater by injecting it into subsurface and extracting in time of need is the principle of an aquifer thermal storage (ATES) system. This technique of energy conservation leads to energy savings, reduction of dependency on fossil fuels and thus reduction in greenhouse gas emission. This study presents a numerical model of an ATES system to store thermal energy and evaluates its performance. A thermo-hydrogeological numerical model for a confined ATES system is presented in this study [1]. The numerical simulations have been performed by the software code DuMux [2]. The model takes into account heat transport processes of advection, conduction and heat loss to confining rock media, regional groundwater flow in the aquifer, geothermal gradient and anisotropy in the aquifer. Thermal interference in the system when the thermal-front reaches the production well affects the system performance and hence should be avoided. This study predicts the transient temperature distribution in the aquifer for different flow and geological conditions. This may be effectively used in designing an efficient ATES project by ensuring safety from thermal-breakthrough while catering to the energy demand. Based on the model results a safe well spacing is proposed. The thermal energy discharged by the system is estimated.The present numerical model is also found to approximate the results of an experimental field study quite well.

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Transient Temperature Analysis for Characterization of Multilayer Reservoirs with Crossflow

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Multilayer system as a result of the sedimentary deposition process is widely existing in underground hydrocarbon reservoirs. To obtain accurate multilayer properties and understand the flow behavior in a multilayer system, many testing and analysis procedures have been evolved. In this work, we develop an analytical solution to determine the individual layer temperature signal associated with constant rate production of slightly compressible fluid from a fully penetrating vertical well in a multilayer reservoir. The analytical solution development process involves identifying the late time individual layer production rates and applying the single layer transient temperature behavior, the results of which are benchmarked with those from the numerical simulation. The temperature signals are presented at the bottom-hole location and further into the reservoir for two-layered and multi-layered systems, for which each layer can be damaged or undamaged. In addition, we provide semi-log temperature interpretation techniques to characterize the layer permeability and porosity, and damaged zone radius and permeability. The temperature profiles obtained from analytical solution shows excellent agreement with those from numerical simulation and are sensitive to layer permeability, porosity, and damaged zone properties. Sensitivity analyses of temperature profiles are performed on layer properties of permeability, porosity, damaged zone radius and permeability. Higher layer permeability increases the radius of investigation of Joule-Thomson and adiabatic expansion effects by rising speeds of temperature propagation. Porosity variations result in changes of adiabatic expansion effect associated with the heat capacity of the saturated porous medium. The effects of damaged zone radius and permeability on temperature signals are analogs with those produced from a single layer reservoir. With adequate knowledge on other layer properties, detailed procedures are demonstrated and can lead to the interpretations of layer production rates, permeability, and damaged zone permeability for each layer. Even with no prior knowledge of other layer properties, simplified procedures reveal the ratios of layer production rates, permeability, and damaged zone permeability between layers. Field data have been applied on these interpretation procedures to obtain reservoir properties, which are validated with the reference. The analytical solution presented in this paper is the first one to predict the transient temperature signals in a multilayer reservoir so far. These derived interpretation techniques significantly simplify the complications associated with the inversion from numerical simulation while maintaining decent accuracy. Implementing these techniques to downhole temperature measurements has confirmed the field application of this study.

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A new model of single micro-fracture and an empirical flow function

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With the advance of the X-ray computed tomography (CT), the internal structure of fractured rocks is able to be accurately revealed and so the fluid flow through micro-fractures with apertures at mm-/μm-scale has received an enormous attention over the last decade. Due to the two facts that normally fracture voids are bigger than surrounding pores, and the fracture network is well developed, thus it is important to characterise the fracture morphology and investigate the fluid flow in fractures. We develop a new model for single natural fractures and use the fracture model with various parameters to feed in numerical simulators aiming to predict flow and transport properties. The proposed modelling algorithm combines both aperture filtering and local addition/subtraction operation on random numbers, in which the fracture aperture, contact area and roughness are all taken into account. Two rough surfaces, which are spatially correlated in terms of local aperture values and local surface shapes, can be generated not just separately but also simultaneously based on the smoothing (e.g. the maximum and the mean) filters[1], performing on two random arrays, which are utilised as a data structure to describe the two surfaces. The touch-points, forming the contact area of fractures, result from continuous tier corrosion using the local addition and subtraction operation[2]. The variogram and the normalized cross-correlation coefficient are calculation to measure the spatial continuity of fracture surfaces and to quantify the similarity of the two fracture surfaces. And by choosing different combination of model parameters – aperture, roughness and contact area the effect of fracture morphology on fluid flow is further investigated to numerically gain the relationship between microscopic features and macroscopic properties. An empirical formula (function) that correlates fracture permeability with fracture roughness, mean aperture, and contact area is achieved to overcome the big error of using the Cubic law for natural fractures with the Lattice Boltzmann method. As a result, in general the absolute permeability will be reduced more than 20% in comparison to the Cubic law.

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AN EXPERIMENTAL AND ANALYTICAL INVESTIGATION INTO THE EFFECTS FRACTURE–PARALLEL STRESS ON WATER PERMEABILITY FOR A SINGLE FRACTURE

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To address the current vague understanding of the effect of stress on the transport law of fluid flow in fractures (see Zhang et al., 2007; Bai et al., 1999; Yeo et al., 1998; Walsh, 1981), we conducted a series of experiments on single-fracture seepage under true-triaxial stress in the laboratory. It was demonstrated that fracture permeability decreased with an increase in stress parallel to the fracture plane, exactly the applied direction of which was parallel to the direction of the fracture, exactly the opposite to the results of other reports (e.g., Zhang et al., 2007; Bai et al., 1999). Taking into account the effect of normal and fracture-parallel strain on fracture permeability, an analytical formula for the fluid-seepage law for a single fracture under three-dimensional (3D) stress was deduced. The formula shows clearly that the fracture-permeability coefficient will decrease in a negative power relationship with an increase in the sum of normal stress and fracture-parallel stress. The effect of fracture-parallel stress is decidedly less than that of normal stress. It was also found that other parameters, such as the fracture-connectivity coefficient, normal rigidity, the Young's modulus and Poisson's ratio of the intact rock, will affect the fracture-permeability coefficient.

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Calculation of Biot-Willis coefficient and Shear Modulus of a porous medium using pore-network modelling

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Hydraulic fracturing is a promising method for IOR/EOR in unconventional reservoirs. To predict the effectiveness of this process, correct values of geo-mechanical properties of the porous medium is necessary. In addition, these properties have important effects on calculating the rate of fracture propagation and breakdown pressure. Although Biot's theory is a well-received poroelastic theory to involve calculation of geo-mechanical properties of isotropic and homogenous rocks, there exists two degree of freedom for that theory which should be calculated first, Biot-Willis coefficient and Shear modulus. In this study by the use of 3D pore-network modelling, which is a well-known methodology for calculation of absolute/relative permeability, a few analytical expressions are developed for Biot-Willis coefficient and Shear modulus. The results of our study are compared with experimental data for validation. In addition, our results show that Shear modulus can be interpreted as a geometric property. This achievement is practical to improve available commercial softwares, which use pore network modelling, for calculating geo-mechanical properties as well.

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Change in three-dimensional rock mass permeability during the growth of geomechanical fractures

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The impact of fracture growth on the effective permeability of a rock masses is investigated and quantified. The explicitly computed macroscopic permeabilities are compared to the predictions of classical inclusion-based effective medium theories, and to the permeability of networks of randomly oriented and stochastically generated fractures. Stochastically generated fracture networks often lack features that arise from fracture interaction, such as non-planarity, and termination of fractures upon intersection. Recent discrete fracture network studies include heuristic rules that introduce these features to some extent (e.g. Bonneau et al., JGR, 2016). These features may be key to realistically modelling the hydraulic properties of fractured rock. In particular, using fracture networks that are generated using rigorous laws of geomechanics will allow the study of the evolution over time of permeability, as a result of the applied stresses. In the present work, fractures are grown using a fracture mechanics-based simulator (Paluszny & Zimmerman, Eng. Fract. Mech., 2013), extending under tension from a finite set of initial flaws. The finite element method is used to compute displacements, and modal stress intensity factors are computed around each fracture tip using the interaction integral accumulated over a set of virtual discs. Fracture apertures emerge as a result of simulations that honour the constraints of stress equilibrium and mass conservation. The macroscopic permeabilities are explicitly calculated after each step of growth using an upscaling method (Lang et al., JGR, 2014) that solves the local cubic law in the fractures, on an element-by-element basis, coupled to Darcy's law in the matrix. The explicitly computed permeabilities are compared to the predictions of classical inclusion-based effective medium theories (Saevik et al., Transp. Porous Media, 2013) - in particular, the symmetric and asymmetric self-consistent effective medium approximations, which have been shown to work well for isotropic networks (Ebigbo et al., Transp. Porous Media, 2016). The permeabilities of several dozen geomechanically-grown fracture networks are computed as a function of fracture density and in situ stresses. The evolution of effective permeability can be correlated to the applied stress over time. In fracture networks containing many growing fractures, dominant fractures which accumulate more growth also develop larger apertures, leading to flow pathways that significantly enhance the effective permeability. For anisotropic networks, in cases where there is a dominant fracture set, it is found that the asymmetric and symmetric self-consistent methods overestimate the effective permeability in the direction of the dominant fracture set. These effective medium theories are more accurate in cases in which the permeability is controlled by two or more fracture sets.

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Comparison between Analytical and Numerical Methods for Predicting the Length of Hydraulic Fracturing

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During recent decades, the process of hydraulic fracturing has been widely used for the stimulation of petroleum reservoirs. Due to the heterogeneity of material properties, rock structure and in-situ stress state, hydraulic fracturing process is highly complex. As a result, it is difficult to predict or even measure the behaviour of hydraulic fractures in field conditions. In this paper, analytical approaches for predicting the length of propagated fracture consist of PKN, KGD, and radial methods are reviewed. Then, crack propagation was simulated by Discrete Element Method (DEM) in two dimensional space and with considering the plane strain condition. To achieve this aim, a fracture network was modelled with fictitious joint technique. The fictitious joints have a same properties equalled with the intact rock. A Vornoi tessellation scheme (trigon blocks) was used to add the necessary degrees of freedom to model the propagation path of a hydraulically driven fracture. The results showed that the predicted length of hydraulic fracturing in KPN model is more than other methods and numerical results has a good agreement with KGD model. The numerical results also indicated that the hydraulic fracturing is propagated in the maximum horizontal stress.

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Effective coarse-grained properties of fluid-filled fractures

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Interpreting characteristics of seismic waves in fractured porous media is important for various applications like geophysical exploration, oil or gas exploitation or water reservoir management. The significance of the interpretations largely results from systematic modeling of wave propagation. In the present contribution, we discuss effective hydro-mechanical properties of reservoir rocks on the REV scale as derived from computational homogenization [3, 4]. Fracture networks in a perodic unit cell are stochastically generated mimiking typical reservoir scenarios. The resulting fluid-filled (fractured) poroelastic rock is numerically investigated by Finite Element Methods. For fractures with high aspect ratios, numerically efficient hybrid-dimensional discretization schemes are developed [1].

From the numerical results in the time-domain, we determine an effective pseudo-Skempton coefficient us- ing computational homogenization approaches to replace the heterogeneous Biot medium by a macroscopic, homogeneous viscoelastic substitute medium [2]. The pseudo-Skempton coefficient captures two viscous at- tenuation phenomena, pressure diffusion parallel to the fractures and leak-off perpendicular to the fractures. The two attenuation mechanisms are caused by viscous solid-fluid momentum interaction but are related to different inherent diffusion lengths and characteristic times (or frequencies). We show, that the analysis of the pseudo-Skempton coefficient in frequency space provides a valuable tool for the discussion of interconnectivity of fracture networks and for the determination of aspect ratios of fractures in reservoirs.

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Fractured Porous Media in Diagenetic Geological Environment; Effects on Fluid Flow

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The intrinsically low permeability in shale may be altered by diagenetic changes in internal surface properties. The effective permeability of any porous medium is largely a function of its global fractured and non-fractured geometry. The estimation of dimensionless quantities such as Peclet (Pe) and Peclet-Damkohler (PeDa) Numbers that were associated with geochemical reactivity of rocks and acidic fluid transport through porous media have previous given insights into the impact of diffusion and reaction rate on shale caprock in CO2 sequestration. As reported in the literature, nano-scale measurement of changes in internal specific surface area, pore volume and linear/cumulative pore size distribution (using the BET Technique) showed that changes in the shale caprock due to geochemical interaction with aqueous CO2 can affect petrophysical properties. It is also known that the mineralogical components of sedimentary rocks are geochemically active particularly under enormous earth stresses, which generate high pressure and temperature conditions in the subsurface. It has been postulated that the effect of mineralization can lead to flow impedance in the presence of favorable geochemical and thermodynamic conditions. Simulation results suggested that influx-induced mineral dissolution/precipitation reactions within clay-based sedimentary rocks can continuously close micro-fractured porous networks, though injection pressure and effective-stress transformation first rapidly expand the fractures. This experimental modelling research investigated the impact of in-situ geochemical precipitation on conductivity of fractured porous media under geomechanical stress conditions. Geochemical analysis were performed on different samples of shale rocks, effluent fluids and recovered precipitates both before and after CO2-brine flooding of crushed shale rocks at moderately high temperature and pressure conditions. Differential pressure drop data across fractured composite core were also measured with respect to time over a five day period. This was used in estimating the conductivity of the artificially fractured cores. Three experimental runs per sample types were carried out in order to check the repeatability of observed changes. The results showed that most significant diagenetic changes in shale rocks after flooding with CO2-brine, reflect in the effluent fluid with predominantly calcium based minerals dissolving and precipitating under experimental conditions. Major and trace elements in the effluent fluid (using ICP-OES analysis) indicated that multiple geochemical reactions are occurring with almost all of the constituent minerals participating. The geochemical composition of precipitates recovered after the experiments showed diagenetic carbonates and opal (quartz) as the main constituents. The bulk rock showed little changes in composition except for sharper and more refined peaks on XRD analysis, suggesting that a significant portion of the amorphous content of the rocks have been removed via dissolution by the slightly acid CO2-brine fluid that was injected. . The differential pressure drop, its 1st order derivative and estimated fracture conductivity indicated that reactive transport of dissolved minerals can occlude micro-fracture flow paths, thereby improving caprock seal integrity with respect to leakage risk under CO2 sequestration conditions. Diffusive transport of CO2 as well as carbon accounting could be significantly affected over the long term.

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Geomechanical Damage of Naturally Fractured System Due The Stresses Induced By Production Fluids

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When a formation is drilled a redistribution of the stress around the well is generated, triggering a decrease in the permeability (Geomechanical Damage –GD) of the naturally fractured system. This has sparked interest in the industry and it has allowed the development of several techniques of static characterization as well as their deformability by stress state (dynamic characterization). The opening, orientation, spacing, frequency, geometry and shape are the most common static attributes of natural fractures. Studies on the deformability of fractures by stresses have been limited and made under ideal conditions that do not represent the in-situ stress state of the well. In order to mitigate the geomechanical damage is necessary to understand the dependency of deformability of fractures with stresses to in-situ conditions. An optimal diagnosis allows a good understanding of the relationship between the spatial and temporal variability of the permeability on the natural fractures. This study develops an analytical model that couples the static attributes of natural fractures, the geomechanics rock properties and the stresses around the well with natural fractures deformability models. The model is used to study the impact of the geomechanic damage on the well productivity and its affectation ratio. Additionally, through an analysis of sensitivity, most affected parameters on the geomechanical damage are identified (For example: Natural fractures orientation, natural fractures opening, stresses orientation, resistance and elastic properties of the rock, anisotropy stresses, stress around the wellbore, wellbore path, etc.). The study shows that the geomechanical damage caused by the stress induced due to fluids production in naturally fractured systems is not a function of a single variable. The permeability of the natural fractures is a function of the stresses around the well, the geomechanical properties of the formation, the static attributes of natural fractures and the stress state, among others. The integrated study of these factors constitute an optimum methodology to diagnose the geomechanical damage in naturally fractured systems.

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Gravity-driven control of the spatial distribution of calcium carbonate precipitates in a fracture

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Sealing fractures by mineral precipitation is an important process for improving caprock integrity in subsurface reservoirs. We investigated the effect of buoyancy and fracture orientation on the amount and spatial distribution of calcium carbonate (CaCO3) precipitates in a fracture model. To monitor CaCO3 mineral precipitation during reactive flow, transparent acrylic casts of an induced fracture in Austin chalk were used. To induce pore-filling CaCO3 precipitation, 1M CaCl2 and 0.3M Na2CO3 were injected simultaneously into a fracture replica saturated with the sodium carbonate solution. Experiments were performed with the fracture plane oriented either parallel or perpendicular to gravity. Acoustic wave transmission (compressional wave, 1 MHz) and optical imaging were used to monitor the sample prior to, during, and after fluid injection. Complementary X-ray computed tomography was performed throughout the experiments real-time on vertical fractures and for the horizontal fractures, post injection tomography measurements were conducted. When the fracture plane was oriented parallel to gravity, the denser CaCl2 solution almost completely displaced the sodium carbonate solution in the fracture and caused strong localization of the precipitates. The width of the precipitated region grew slowly over time. When the fracture plane was oriented perpendicular to gravity, the less dense sodium carbonate flowed over the CaCl2 solution thus resulting in more mixing and a more uniform distribution of precipitates throughout the fracture plane. By adjusting the density contrast between the two solutions, the spatial distribution of precipitates in a fracture can be controlled and localized to different regions of the fracture plane. The potential to improve caprock integrity through induced mineral precipitation must account for gravity-driven chemical dynamics that can result in differences in the amount and spatial distribution of precipitates among horizontal and vertical fractures. This work was supported by the Center for Nanoscale Controls on Geologic CO_2 (NCGC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-AC02-05CH11231

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Modeling of fracture propagation at reservoir scale and coupling with reservoir fluid flow

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It is well-established in the oil & gas industry that many operations of waterflooding and EOR take place under high pressure injection conditions such that induced (hydraulic) fracturing occurs [1]. From reservoir simulation perspective having new fractures in the reservoir can significantly change its flow pattern even leading to unintended short-circuiting between injectors and producers. The geomechanics of the fracturing process in its turn can lead to such risks as activation of existing faults and generation of earthquakes. To make a reliable assessment of the above risks, one needs a coupled fracture-reservoir simulation capacities. Within such a framework, accurate modeling of the fracturing process requires high resolution both in space and in time. It is not possible to provide such resolution in a conventional reservoir simulator and an application of a multi-scale technique is required. The technique we use in this study combines the Discrete Fracture and Matrix (DFM) model [2] with the contact-plane geomechanical [3] model that was recently proposed for modeling the naturally fractured reservoirs. In this technique, the flow equations are approximated by finite-volume method and the mechanics equations are discretized by means of Galerkin finite-element approach. The mechanical behavior of the fracture is modeled as a contact problem between two finite elements. The most of the fractures are inactive from the beginning and are being activated and widened throughout the simulation. The pressure wave propagating through the domain opens the new fractures by triggering the opening criteria. The open fracture adds an extra volume into the DFM formulation. The set of fully coupled equations is solved implicitly at every simulation step. We are testing the proposed model against well-known (semi-) analytical solutions for simple systems [4]. Apart from that, in the scope of this project we consider the ranges of applicability both in terms of effective model parameters and resolution of discretization in space and time.

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Simulation of fracture dissolution in rocks: three-dimensional approach

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Typically, numerical models of fracture dissolution are simplified and represented by the system of one or two-dimensional fields. These approaches can explain many observations in nature, like the estimation of the breakthrough time or formation of the wormholes (highly localized flow paths). However, such modeling is limited to the early stages of fracture dissolution where the variations in aperture are small. As the dissolution patterns develop, a 2D model is unable to correctly capture the flow in the vicinity of the wormholes and tends to overestimate the degree of competition between adjacent flow paths [Starchenko et al., 2016]. At this point a three-dimensional simulation is needed to correctly capture the flow and reactant transport. We have found that elliptically shaped channels can develop very early on, even before breakthrough, when the aperture is in the millimeter range and the flow is still at low Reynolds number. There are qualitative differences in the aperture evolution after breakthrough, depending on whether the flow rate was limited externally or by the viscous drag on the fracture surfaces. At constant pressure drop after breakthrough the fracture tends to dissolve uniformly across its whole width. In case of limited flow rate well-developed conduits have been observed. When the flow rate is low, almost all the reactant is consumed within the dominant conduit, which enlarges without affecting the surrounding fracture matrix. When the flow rate is higher the consumption of reactant in the conduit is limited by the surface reaction rate, and the remaining reactant is available to dissolve the surrounding matrix. Moreover, in case of limited flow after breakthrough bending of shorter channels toward the dominant one (Fig.1C) has been observed.

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Simulations of fracture dissolution in three dimensions

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Fractures take up only about 1% of the subsurface pore space, but in soluble rocks they make the most important contribution to groundwater transport; for example in the development of karst formations. The increase in permeability due to dissolution of the fracture surfaces gives rise to a number of questions that are important for waste storage systems, sequestration, oil and gas recovery, and dam stability.

Fractures are usually represented by an aperture field, with the three-dimensional equations for flow and transport replaced by averages over the local aperture. We have examined the validity of this approximation by comparing results from aperture-averaged models with three-dimensional simulations, where the motion of the dissolving surfaces is explicitly accounted for. We find that an aperture-averaged model does not correctly describe the flow in the tube-like conduits that develop as the fracture dissolves, nor does it correctly capture the mass transfer from bulk solution to the dissolving surfaces.

We have used three-dimensional simulations to investigate the dissolution of individual fractures, going past the point where reactant first reaches the outlet and investigating the subsequent development of the primary flow path. We have found that elliptical conduits evolve very early in the dissolution, even prior to breakthrough. They can be nucleated from local enhancements of aperture, from spatially random aperture distributions, or even from variations in the central plane of an otherwise smooth fracture. The shape of the conduit depends on flow rate: at small flow rates they are circular, but expand horizontally into elliptical shapes as the flow rate increases.

We have found significant differences between fractures dissolving under constant flow rate (typical of laboratory experiments) and fractures dissolving under a constant pressure drop, possibly coupled with a flow rate limit (more typical of field conditions). The nucleation of localized flow paths leads to large increases in flow rate through the fracture, particularly when there is an ample supply of water.

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Solute transport, flow connectivity and biofilm growth in fractured media: field observations from multiscale tracer tests, geophysical imaging and genomic sequencing

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Transport processes in fractured media and associated biogeochemical reactions are governed by multiscale heterogeneity ranging from fracture wall roughness at small scale to broadly distributed fracture lengths at network scale. This strong disorder induces a variety of emerging phenomena, including flow channeling, anomalous transport, enhanced mixing and biofilm development. These processes are generally difficult to isolate and monitor in the field because of the high degree of complexity and coupling between processes, and the difficulty to obtain representative datasets. We report in situ experimental observations from the Ploemeur fractured rock observatory (http://hplus.ore.fr/en/ploemeur) that provide new insights on coupled flow, transport and reactions phenomena in fractured media.

The presented dataset includes multiscale dipole and push pull tracer tests that allow understanding and modelling anomalous transport processes characterized by heavy-tailed breakthrough curves (Kang et al. 2015), and time lapse Ground Penetrating Radar monitoring of saline tracer tests that provide a dynamic characterization of the distribution of transport pathways at network scale (Shakas et al. 2016). The vertical connectivity of such fracture networks is shown to induce rapid oxygen delivery and mixing at depth leading to biofilm development. Through genomic sequencing of bacterial populations at different depths, we discuss the link between fracture connectivity, transport processes and microbial diversity. Hence, this presentation will attempt to link experimental observations made at different scales to quantify and model the coupling between flow channeling, non-Fickian transport, mixing and biogeochemical reactions in fractured media.

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The first-order slip-corrected Reynolds equation and the upscaled model for slightly compressible gas flow in a fracture

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Pressure-driven gas flow between confined rough walls is a common situation arising in many industrial applications ranging from fluid recovery through fractured rocks to leak rate determination of static seals. In these applications, the transport properties of the fractures represent a critical issue as it can determine the success or failure of the system. A real rough fracture is usually characterized by an heterogeneous and multi-scale aperture field along with localized contact spots. A direct modeling of the transport properties of this connected topography can therefore be a very challenging task.

In this work, we study the slightly compressible flow of a gas in the slip regime [1] within a rough, heterogeneous fracture. Starting from the governing Navier-Stokes, continuity and state-law equations along with a first-order slip boundary condition at the walls of the fracture, the two-dimensional slip-corrected Reynolds model is first derived. It is shown to be first-order accurate in the Knudsen number while being second-order accurate in the local slope of the asperities.

In a second step, the focus is laid upon the flow-rate to pressure-gradient relationship over a representative aperture element of the fracture. For this purpose, an upscaling procedure is applied to the local Reynolds equation by making use of the volume averaging method [2]. This yields a macroscopic flow model in which the momentum conservation equation has a Reynolds-like form that relates the mass flow-rate per unit width of the fracture to the pressure-gradient involving a so called transmissivity tensor. The effective macroscopic transmissivity tensor, characteristic of the representative aperture element, is shown to be given by a closure problem that is not intrinsic in a sense that it depends not only on the geometry of the aperture field but also on a slip parameter. However when the slip effect is neglected, the closure problem becomes intrinsic and recovers previous models from the literature [3], thus yielding the intrinsic transmissivity tensor of the representative element.

Comparisons between results obtained from direct numerical simulations at the microscale and predictions from the solution of the closure problems are performed on case examples.

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Thermally Induced Fractures during Heat Extraction from Geothermal Doublets

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Heat extraction from geothermal doublets is becoming a promising source of energy in near future. In low permeability geothermal reservoirs, fracturing in injection and production wells is needed to improve injectivity and productivity of the wells. Fractured geothermal doublets are susceptible to short-circuiting, in which the residence time of the fluid is shorten, leading to reduced efficiency of the geothermal system. Cooling down of the rock matrix due to the heat extraction, results in a volume change of the matrix and aperture variation of the fractures. The combined effects of temperature and fluid pressure variation in subsurface can contribute to creation of new fractures as well as propagation of present fractures (induced or natural fractures). Such thermal fracturing has been observed in water injection wells in petroleum industry (Bellarby, 2009) and in geothermal wells (Benson et al, 1987; Tulinius et al, 2000). In the present work, a three-dimensional finite-element model has been utilised to simulate the heat extraction from a fractured geothermal doublet. In present model, the fractures are modelled as discontinuity surfaces within 3D rock matrix. The fluid flow and heat transfer within the fractures and the rock matrix are coupled with mechanical deformation of the matrix. The fracture aperture variation is directly computed from mechanical deformation of the rock matrix. The growth of fractures is modelled using the concepts of linear elastic fracture mechanics (LEFM), with the onset and direction of growth based on stress intensity factors. This model has been verified against several analytical solutions available in the literature. A sensitivity analysis on the injection parameters such as injection rate, and fluid temperature has been performed to investigate the effects of thermally induced deformation of the rock matrix on the growth of fractures in the geothermal doublet.

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Chromatographic analysis of the salinity-acidity system

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Salinity in aqueous systems governs electrostatic behavior of dissolved ions and charged surfaces. These phenomenon are well understood in batch settings, yet their influence on transport behavior is not. Of primary concern is the coupling of salinity and acidity through reactive surfaces. Saline intrusion is often modeled with ion exchange, yet changes in pH are seldom reported and a full analysis of the role of surface chemistry models has not been presented. To gain insight we extend chromatographic theory to the salinity-acidity system including the most common surface chemistry models. Transport predictions are then compared against a systematic set of column experiments through silica sand. The analysis shows salinity can induce an order of magnitude change in acidity, even in the absence of salt sorption. The direction and magnitude of this change is only captured when both the Helmholtz and diffuse layer components of the surface electrostatic model are considered. The ion exchange model is therefore a poor representation of the underlying physical phenomenon in such systems and a full surface complexation model is needed.

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Classification of cross-diffusion-driven convection in 3-component double-layer systems: theory and experiments.

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Cross-diffusion [1], whereby a flux of a given species entrains the diffusive transport of another species, can trigger buoyancy-driven hydrodynamic patterns at the interface between initially stable stratifications [2,3,4]. We describe this phenomenon by means of a 3-component (1 solvent and 2 solutes) cross-diffusion-convection (CDC) model where fickian diffusion (including cross-diffusion terms) is coupled to Stokes equations [2].

In order to isolate the sole effect of cross-diffusion in the destabilization of a double-layer system, we impose an initial concentration gap of one solute in the bottom layer while the other component is homogeneously distributed over the spatial domain. We show that we can selectively promote two possible types of hydrodynamic scenarios (negative cross-diffusion convection, NCC, and positive cross-diffusion convection, PCC) corresponding to the cross-diffusive influence (i.e. positive or negative) of the heterogeneously distributed solute on the homogeneous one.

The study of the space-time density profiles along the gravitational axis allows us to derive analytical conditions for the onset of these instabilities as a function of two important parameters: the cross-diffusion term and the buoyancy ratio, giving the relative contribution of the two species to the global density. The general classification of the NCC and PCC scenarios in this restricted parameter space is supported and complemented by numerical simulations of the fully nonlinear CDC problem.

The spatio-temporal convective dynamics obtained from simulations compare favourably with experiments performed with AOT water-in-oil reverse microemulsions (ME) [3], in which initially stable stratifications between two ME with a different composition are studied in a Hele-Shaw cell. Thanks to their characteristic compartmentalized structures at the microscopic scale, ME are able to induce both macroscopic convective modes predicted in the general theory. Indeed, while PCC scenarios have been already found experimentally in previous works [4], NCC modes are isolated here for the first time by using ME.

We briefly discuss how cross-diffusive convection can be exploited to destabilize statically stable stratifications in the context of pollutant remediation, to promote the transport of incapsulated chemical information in response to a given chemical gradient (drug-delivery) and to increase the mass transfer rate. ME are also analyzed as a convenient model system for future studies on pattern formation arising from the interplay between cross-diffusion-driven convection and chemical reactions [1].

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Disproportionate Permeability Reduction (DPR) Process Evaluation in One of the Iranian Oil Reservoir while Gel Polymer Flooding

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Water production is one of the serious problems in production of oil and gas reservoirs. Water coning in oil wells not only causes oil production reduction, but also increasing separation costs and equipments maintenance. Above all in many cases caused the oil production cut off and much oil remain in the reservoir that is not producible. Nowadays, the use of gel polymers becomes very important due to prevent water and gas production in oil wells and water production in gas wells. One of the reasons that make gel polymer's performance become successful is its ability to reduce water permeability more than oil permeability that this phenomenon is called disproportionate permeability reduction (DPR). This research is laboratory survey of gel polymer's performance order to prevent water producing in enhanced oil recovery (EOR). In this study, two series of experiments were performed on different samples. The first series includes three phase experiment on plug and the second series includes four phase experiment on core samples. It is explained that the gel polymer compositions will differ with each other during different steps of experiments. The results show that the gel polymer seal time and the viscosity of gel polymers are two fundamental factors in experiments. Because, if gel polymers do not have suitable seal time could not be diffused in to the fractures and was sealed before reaching the region was fractured by water. Also, if the gel polymer composition does not have suitable viscosity, many problems would happen during water injection. These problems include pressure increasing (due to high viscosity) and production in injection wells (due to low viscosity).

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Effect of electrostatic interactions on pH fronts propagation in saturated porous media

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Electrostatic interactions and molecular diffusion have been increasingly recognized as important factors for the transport of ionic species in porous media. Such processes affect the displacement of charged species in pore water under both diffusion-dominated [1] and advection-dominated flow regimes [2]. This work presents an investigation of pH fronts propagation during multicomponent ionic transport in saturated porous media under flow-through conditions. We performed laboratory bench-scale experiments and numerical modeling to show the important influence of Coulombic effects on proton transport in the presence of ionic admixtures. The experiments were performed in a quasi two-dimensional flow-through setup under steady-state flow and transport conditions. Dilute solutions of HCl with MgCl2 (1:2 strong electrolyte) were used as tracer solutions to experimentally test the effect of electrochemical cross-coupling on the migration of diffusive/dispersive pH fronts. We focus on two experimental scenarios, with different composition of tracer solutions, causing remarkably different effects on the propagation of the acidic fronts. We observed relative differences in the penetration depth of pH fronts of 36% between the two scenarios and of 25% and 15% for each scenario with respect to the transport of ions at liberated state (i.e., without considering the charge effects). Also significant differences in the dilution of the distinct ions plumes, quantified using the flux-related dilution index at the laboratory bench scale [3], were measured at the outflow of the flow-through system. The dilution of the pH plumes also changed considerably (26% relative difference) in the two flow-through experiments only due to the different composition of the pore water solution and to the electrostatic coupling of the ions in the flow-through setups. Numerical transport simulations were performed to interpret the laboratory experiments. The simulations were based on a multicomponent ionic formulation accurately capturing the Coulombic interactions between the transported ions in the flow-through system. The results of purely forward simulations show a very good agreement with the high-resolution measurements performed at the outlet of the flow-through setup and confirms the importance of charge effects on pH transport in porous media.

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Effect of salinity and temperature on pH-dependent transport of heavy metals and radionuclides in reactive porous media

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Hydraulic fracturing (or fracking) is a well stimulation technique for unconventional oil and gas extraction [1]. Around 8-38 million cubic meters of fracking fluid containing water, chemicals, and proppant are injected into the shale every day [2]. High-pressure injection of the fracking fluids fractures allows the gas and oil to be mobilized and flow towards the surface. Together with the gas, the formation hypersaline brine (i.e., the flowback and the produced water) containing heavy metals and radionuclides, such as barium, strontium, and radium, is extracted. Spills of flowback and produced water into the subsurface may occur during operation, handling, and storage with potential negative impact on potable aquifers. Salinity reduced adsorption because of the compression of the double layer of a liquid-solid interface. But, the degree of the reduction of the adsorption of the heavy metals and radionuclides at the hypersalinity of the brine has not been studied, yet. Here, we present an experimental and modeling work to describe the effect of salinity, pH, and temperature on the transport of the major cations present in the produced water. We selected a porous medium containing goethite as it is a common mineral in shallow aquifer and we created a synthetic brine upon the characterization of Marcellus shale produced water. We measured adsorption isotherms and, then, performed column-flood experiments systematically changing salinity, pH, and temperature within the conditions of interest. Preliminary results on barium show that adsorption becomes significant above pH 7, but decreases with salinity and temperature, being negligible at the upper salinity value of produced water, i.e., 3 m. In particular, we observed that with the increasing salinity, the adsorption of barium decreases significantly from 70% to 30% of the initial concentration. Column-flood experiments under conditions at which adsorption of barium was still expected, i.e., pH 8 and salinity of 1 m, show no retardation of the metal, but rather a travel speed equal to average flow velocity (Figure 1.a). Similar transport might be expected for radium and strontium as they have a chemical behavior similar to barium (Figure 1.b). This suggests that in a case of a spill of produced water within an aquifer containing iron-oxide mineral, a fast migration of the major metals and radionuclides may occur with a potential negative impact on aquifer water quality.

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Fast pH-dependent transport of heavy metals and radionuclides due to longitudinal and transverse dispersion

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Leakage of radioactive wastewater temporally stored in underground tanks can lead to the escape of heavy metals and radionuclides into the subsurface. Several measures have been taken to reduce the risk that such event may happen. One example is the addition of chemicals into the wastewater that raise the pH to basic. As alkaline conditions favor the adsorption of heavy metals and radionuclides on common mineral surfaces (e.g., iron oxides, aluminum oxides, clays and carbonates) retarding significantly their transport[1]. However, observations show that heavy metals and radionuclides within an alkaline solution can travel much faster than expected when the leakage occurs into an aquifer with acidic pH [2]. This phenomenon was shown for several heavy metals and radionuclides in our earlier work [3]. It occurs because mixing induced by longitudinal hydrodynamic dispersion creates a low-pH zone within the reactive porous medium, favoring the formation of a fast contaminant pulse (or wave) that travels at the average groundwater velocity. Earlier field observations showed that transverse dispersion may also favor the pH-dependent fast transport [4].

Here, we show numerical simulations and experiments of fast pH-dependent of strontium (Sr^{2+}) transport induced by both longitudinal and transverse dispersion. We performed experiments using a bead-pack containing activated alumina (Al_2O_3), selected on the basis of its significant Sr^{2+} adsorption above pH 7 (Figure 1) and its white color, that allows to visualize well the pH plume with a pH-sensitive dye (Bromophenol Blue). In preliminary tests using glass beads under the conditions of interest, the description of the pH plume with high-resolution images agrees with the chemical analyses at the outlet. Currently, we are performing experiments to verify our numerical simulations shown in Figure 2, which are performed under the conditions favoring fast pH-dependent transport, i.e., initial acidic pH in the system, followed by the injection in the lower half of the domain of a basic solution containing Sr^{2+}.

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Nanoparticles for Permeable reactive barriers: Production and application of mobile particles

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Permeable reactive barriers have been recognized as a cost-effective technology for in-situ groundwater remediation. Placement of the barrier underground is the biggest challenge in this technology, consuming most of scientific and financial resources, so far. Injecting engineered nanoparticle suspensions to create a reactive barrier in soils has shown potential to overcome this challenge. Nanoparticles will deposit on aquifer sand, and then adsorb and/or react with groundwater contamination. Injection can be made using wellbores, thus reducing the costs of the barrier placement. However, nanoparticles have low mobility and are transformed (and thereby lose their capacity to react) in the close vicinity of the injection zone. We have designed and produced Goethite nanoparticles to adsorb heavy metals in contaminated groundwater. Our colloidal suspensions show high stability and mobility in different sediment types. Laboratory tests with aquifer materials and numerical simulations were combined in order to understand how different hydrological and hydrogeochemical parameters affect the particle mobility when injected in porous media. The final nanoparticles are stable over days, facilitating transport from the place of production to the injection sites, and therefore minimizing on-site modification. By adjusting the concentrations of the injected suspensions and the injection flowrates, a desired mass of nanoparticles can travel in aquifers without accumulating near the wellbore or clogging pores. For example, a radius of influence of 4 meter was achieved at an injection rate of 60l/min. At such scale, the number of drilling and completion activities are lowered and stable, cost-effective reactive barriers can be placed. We thus present an applicable technology for the creation of in situ adsorption barriers for heavy metals in groundwater.

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Pore-scale modelling of multispecies reactive processes: impact of physical and chemical heterogeneities studied on pore-space images

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Laboratory measurements of mineral dissolution rates differ from those observed in field-scale natural systems [1]. In order to shed light on the source of this discrepancy, we carry out numerical simulations at the pore scale using micro-CT images. While previous works in this area used a particle-tracking method to simulate single-species transport and dissolution of chemically homogeneous rocks [2], this work proposes a methodology that can simulate fluid-fluid and fluid-solid multispecies reactive transport through chemically heterogenous rocks. This methodology allows us to assess the combined effect of physical and chemical heterogeneity on the evolution of dissolution and precipitation.

We simulate multispecies reactive flow directly on voxelised pore-space images obtained from X-ray microtomography (Figure 1). We couple a Stokes-flow and advection-diffusion transport solver to a multispecies geochemical solver [3] using a sequential non-iterative approach. This methodology permits pore-by-pore comparison with laboratory experiments on micro-CT images and can be used to study the interplay of physical and chemical heterogeneities at the pore scale.

From the initial pore-space geometry, we calculate the steady-state velocity field using a finite volume method. Then, we solve the advection-diffusion equations for the concentration fields. Finally, a chemical equilibrium and kinetics problem is solved for each pore voxel, which is considered as a well-mixed batch with an added solid phase if the pore voxel is in contact to a solid voxel. Using this approach, both fluid-fluid and fluid-solid reactions are considered. As dissolution and precipitation takes place, the geometry is changed and the velocity and concentration fields are updated accordingly. The chemical heterogeneity is taken into account by associating each solid voxel to a different mineral and its respective reaction rate.

The geochemical solver is specifically designed to handle sequential equilibrium problems like the ones that arise from the perturbation of the concentration fields by the advection and diffusion of species. It assumes that reactions can be classified into fast reactions, which are considered to be in equilibrium, and slow reactions, considered to be controlled by kinetics. Our methodology inherits this assumption, which simplifies the problem by replacing the slow-reactions differential equations with algebraic ones.

We validate the proposed methodology by comparing the analytical and simulated solutions for the dissolution of (a) a solid spherical particle and (b) a fracture modelled as two parallel plates. We compare the model predictions with laboratory experiment of the fluid-fluid reactive transport along a cryolite column [4], and we demonstrate the impact of chemical heterogeneity on the effective reaction rates in a fracture.

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Simulating hydration and dehydration reactions of thermochemical materials in packed bed reactors

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A promising heat storage concept for domestic applications is based on thermochemical materials (TCMs). Major advantages of TCMs compared to sensible heat storage and phase change materials (PCMs) are high energy densities and a nearly loss-free heat storage period. TCMs are used in packed-bed reactors connected to a humidifier. Heat is stored during dehydration of the material, and released during hydration with water vapor. Despite the high theoretical energy density of TCMs, experiments in packed-bed reactors show a lower energy density of up to 60% [1]. In this study simulations on packed-bed reactors are performed and the hydration and dehydration reactions are studied to enhance knowledge on the effective energy density within a reactor [2]. Figure 1 shows typical results of the temperature and velocity field. Moist air is injected at the left side of the geometry. The particles are heated gradually when the hot air flows into the packed bed. The velocity profile is influenced by the particles and the porosity. Different reactor geometries, materials and conditions will be analyzed and based on the results, improvements for enhancing the energy densities will be suggested.

Figure 1: (a) Temperature field (K) of the moist air flow at t = 123 min; (b) Velocity field (m/s) of the flow (u0 = 0.1m/s, p(H2O) = 13mbar, N = 20, kh = 1°C/min, Δt = 10s) [2]

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Theory of precipitation and dissolution through wave analysis

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Precipitation and dissolution of components from/to a fluid play a major role in many different processes e.g. leach mining, transport of metals in aquifers and water injection for oil recovery. When an unsaturated liquid passes over a soluble solid, solid particles dissolve in the fluid. Conversely, if the liquid is over-saturated with a component solid particles form and precipitate. During water flooding, a secondary oil production mechanism, sea water is injected into the reservoir to displace the oil. Due to the difference in the chemical composition of sea and formation water, this approach is prone to scaling, i.e. the formation of precipitates (scales). Scales can occlude the flow and impede production of hydrocarbons and require costly remediation strategies. Understanding the nature of this reactive flow phenomenon and the provision of tools to simulate relevant scenarios is hence paramount for an economic water flooding in mature reservoirs and/or at low oil prices. Due to the long duration and large spatial extent of the problem, the non-linearity of chemical reactions and the intrinsic dispersion in numerical methods, as well as geological uncertainties, conventional discretisation techniques fail to provide accurate result at reasonable computational costs. Here, we address this problem by analysing the wave structure of the problem using methods from the theory of hyperbolic partial differential equations. We focus on the mixing of two reactive fluids in a porous medium with variable porosity. The reactions consist of precipitation and dissolution of minerals. The precipitates are salts that form by reaction of mobile dissolved ions in the fluid. We solve the model by analysing the wave structure of the chemical fronts. We show that the fastest waves propagate with constant porosity while the slowest waves travel at a fixed concentration. In addition, a proof for the uniqueness of the solution is provided. The results indicate interesting phenomena of the co-ion effect such as precipitation of minerals which are not precipitated in either of the two fluids before mixing. Moreover, we show that the intermediate porosity can never be less than that of the two end-points. While this problem was previously tackled using coherence law and composition paths, we reformulate and approach the problem with a rigorous mathematical perspective. In addition, we account for the volume of the precipitate and hence any porosity variations.

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Transient solute transport with sorption in Poiseuille flow

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Previous work on the effect of sorption on solute transport has reached apparently contradictory conclusions. Some authors have concluded that sorption increases the mean solute transport velocity and decreases dispersion relative to a tracer [1], while others have concluded the opposite [2]. Here we resolve this apparent contradiction by deriving a series solution for transient solute transport with sorption in Poiseuille flow, which recovers previous results in the appropriate limits. This solution shows a transition in solute transport behavior from early to late time that is captured by the first and zeroth order terms in the solution. Mean solute transport velocity is increased at early time and reduced at late time, while solute dispersion is initially reduced, but shows a complex dependence on the partition coefficient k at late time. In the equilibrium sorption model, the time scale of the early regime and the duration of the transition to the late regime both increase with log(k), in the limit of large k. The early regime is more pronounced in strongly-sorbing and advection-dominated systems (k >>1, Pe>>1), while it may be absent if sorption is weak or transport is dominated by diffusion (k<<1, Pe<<1). The kinetic sorption model shows a similar transition from the early to the late transport regime and recovers the equilibrium results when adsorption and desorption rates are large. As the reaction rates slow down, the duration of the early regime increases, but the changes in velocity and dispersion relative to a tracer diminish. In general, if the partition coefficient k is large, the behavior in the early regime is well characterized by the analysis of the limiting case without desorption.

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Use of functionalized nanoparticles to selectively control permeability in porous media

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There is growing interest in methods that enable targeted fluid migration in the subsurface by selectively adjusting the permeability of porous media in situ. Such capability would be beneficial in a variety of applications including carbon capture and storage (CCS) where methods to limit leakage are a major obstacle to more widespread deployment [1]. In CCS, injected CO2 is subject to buoyant forces which cause it to rise, often along the wellbore that was drilled for injection, which can provide a preferential flow pathway to the surface if not completed properly [2]. To address the possibility that this annulus between the well and the surrounding formation can become a major source of leakage, we developed functionalized nanoparticles that could be injected along with the CO2. The nanoparticles would partition to the interface between CO2 and H2O and in the event of a leak would react with the CO2 to form carbonate cements creating a mechanical barrier and blocking buoyant flow of CO2. The reactive nanoparticles could be coated with switchable temperature-sensitive organic polymer coatings that would prevent the core from contacting the fluids until the temperature was low enough. In this context, the natural geothermal gradient in the subsurface provides an effective surrogate for depth to trigger reactivity of the nanoparticles.

In this talk we will report on a variety of experimental and modeling techniques carried out over the past year to characterize this approach [3]. In the lab, we conducted column studies to understand the how both diffusion and advection impact the evolution of these reactions under conditions representative of the deep subsurface. Of particular interest is the interplay between pore wall roughness, flow rate, and precipitation rates and the location of precipitates within the pore network. Experiments were carried out in sintered glass bead porous media and samples were characterized using Scanning Electron Microscopy of the pore walls and X-ray Computed Tomography (X-ray CT) of the pore network to understand the chemical and morphological characteristics of the samples before and after reaction. Both methods reveal clear cementing of the porous media that depends on nanoparticle loading rate and CO2 flow rate. CO2 is both a reactant in the generation of carbonate and it can dissolve the carbonate cements when available in large excess. Permeability measurements of the columns are impacted the most by the injection of the nanoparticles whereas carbonation reactions ensure that the precipitated solid is no longer mobile in the formation. These findings suggest that the nanoparticle coating plays a critical role in both controlling the reactivity of the solid, as originally hypothesized, but also in controlling its mobility through the formation. Complementary modeling work is focused on the development of both 1D reactive transport models and 3D pore network transport models. These models are helping us understand the phenomenological properties of this system and the engineering design principals that are needed to effectively deploy these reactive particles for selective permeability control in-situ.

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Viscous fingering instability in reactive systems

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In a porous medium, understanding the evolution of the interfaces between two miscible fluids, when one fluid displaces the other one is of fundamental importance, especially in applications related to enhanced oil recovery [1], chromatography [2] etc. The interface between the fluids deforms into finger-like patterns leading to a viscous fingering instability, when a less viscous fluid displaces a more viscous one [3]. Reactive systems are able to trigger this instability as soon as the chemical reaction changes the viscosity of the interplaying fluids [4]. In processes like polymer or chemical flooding the onset of viscous fingering affects the sensitivity of the oil production. We theoretically investigate how the fingering instability dynamics are affected by the chemical kinetics. We show that the reaction-diffusion specificities of the chemical front can be used to tune the viscous fingering pattern. The properties of this reactive fingering are obtained by computing onset times, mixing lengths and characteristics of the nonlinear fingering dynamics as a function of the viscosity ratios. The instability dynamics are analyzed for different viscosity profiles and reaction conditions.

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A theory for multicomponent liquid-gas filtration combustion

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We present the theory for multicomponent liquid-gas filtration combustion. Our focus is the recovery of light oil through air injection. The solution of the governing equations is given as a series of travelling waves and we focus on the oxidation wave. We generalize a previous formulation, which considered only two components, for an N component liquid fuel. It is shown that the wave properties, i.e., speed and temperature, are determined from an analysis of an internal singular point in the wave. This singular point is called a resonance point because it is given by the equality between the combustion wave speed and the local saturation (Buckley-Leverett) speed. The properties of the resonance point result in the lighter components of the oil in the upstream side of the wave, while the heavier components are pushed to the downstream side. This unexpected result can shed some light on how the transition between the regimes of low and high temperature oxidation occurs.

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Characteristic times for transport and reaction

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For minerals the equilibrium time in a batch operation can vary between a few seconds and hundred thousands of years. We seek when in reactive transport modelling kinetics can be disregarded and equilibrium can be assumed. Following Knapp (1989) we determine the Pe-Da range where we can disregards kinetics. We consider three regions: and equilibrium region I where the Damkohler number, depending on the concentration, is above 100-10^5, region III below Da<10^-3Pe where reaction can be disregarded and the remaining region II were kinetics needs to be considered. The consequence for numerical modelling in geochemistry will be discussed.

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Combustion enhance recovery of shale gas

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The amount of extracted natural gas from low permeable organic rich shale has increased rapidly over the past decade. The technologies used to improve the permeability of a shale gas reservoir are horizontal drilling and hydraulic fracturing. The potential environmental impact of hydraulic fracturing motivates research aiming at alternative permeability enhancement methods. In this paper the possibility of in-situ combustion to improve permeability is investigated. Two possibilities for the in-situ fuel source are considered, viz., methane or kerogen. A one dimensional model is considered. Under simplifying hypotheses a quasi-analytical solution for the corresponding Riemann problem is obtained. The solution was analysed with parameters that correspond to resonance conditions, i.e., conditions for which the speeds of the heat wave and the combustion wave are equal. We conclude that methane combustion cannot generate enough heat to enhance the permeability. However kerogen, if present in sufficient quantities, makes this possible. We present the set of parameters for which the combustion reaches the optimal temperature to improve the permeability. Finally, the analytical approximations are validated with direct numerical simulations. The pressure distribution in the reservoir and the production improvement by the thermal treatment are calculated with the numerical model.

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Effects of water on light oil recovery by air injection

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We formulate a mathematical model for one dimensional flow with chemical reactions resulting from injection of air into a porous medium initially filled with gas, water and volatile oil. Our goal is to investigate the effect of water and steam on oil recovery, and we do so for a medium pressure air injection process. We show that, when the boiling point of the volatile oil is below or slightly above the boiling point of water, the hot steam region moves upstream of the medium temperature oxidation (MTO) wave (where oil vaporization and combustion occur), while the volatile oil and steam condense at the same location; it leads to considerable improvement of oil recovery by the MTO wave. Remarkably, the recovery curves (recovery fraction vs. time) depend weakly on the initial water and light oil saturations. If the volatile oil boiling point is much higher than the boiling point of water, the steam region moves downstream of the MTO wave. In this case the water effect on recovery is weaker and becomes negative for high water saturations. Numerical calculations suggest the existence of an oil boiling point at which a bifurcation occurs that separates solutions with the steam region upstream or downstream of the combustion zone.

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Four decades of front tracking for flow in porous media

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In 1989, James Glimm and collaborators set up a research program for modeling, simulating and analyzing flow in porous media involving accurate representation of surface of abrupt changes in the flow (shock surfaces). The intention was to model thermal and reactive flow in porous media. A major feature of the methodology was the insistence in finding analytically good approximations for relevant features in the flow, to be included in the computer code, a point of view orthogonal to the popular DNS paradigm. Here we review some of the scientific outcome from this effort, already lasting for almost four decades.

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Interactions between thin fingers in unstable growth processes including viscous fingering and chemical erosion.

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Dissolution of porous and fractured rock can lead to instabilities, where long finger-like channels or ‚wormholes'' are spontaneously formed, focusing the majority of the flow. Formation of those structures leads to a significant increase in permeability of the system, and is thus important in many engineering applications, e.g. in acidization during oil and gas recovery stimulation. In this communication, we analyse this process using two different numerical models (a network model and a Darcy scale one). We show that wormhole patterns depend strongly on the amount of soluble material in the system, as quantified by the permeability contrast k between the dissolved and undissolved medium. For small and intermediate values of k, a large number of relatively thin and strongly interacting channels are formed. The longer channels attract shorter ones, with loops being formed as a result (cf. Fig. 1.). However, for large values of k the pattern gets sparse with individual wormholes repelling each other.

Interestingly, a similar succession of patterns can be observed in viscous fingering in a rectangular network of channels. In such a system, anisotropy of the network promotes the growth of long and thin fingers which behave similarly to wormholes. The attraction rate between growing fingers depends strongly on the viscosity ratio, I. The latter plays a role similar to that of permeability ratio for dissolution of porous material (cf. Fig. 2.). To explain this behaviour, we have created a simple analytical model of interacting fingers, allowing us to quantify their mutual interaction as a function of finger lengths, distances between them and - most importantly - relative permeabilities. The theoretical predictions are in a good agreement with simulation data for both dissolution and viscous fingering processes.

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Linear and nonlinear Robin boundary conditions for advection-diffusion using the lattice Boltzmann method

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The lattice Boltzmann method has proven to be a useful numerical method for simulations in porous media. Although less common, the method is also applicable to advection-diffusion problems. In a recent work [1], a method to implement general flux (Robin) boundary conditions using the lattice Boltzmann method has been developed. The boundary conditions provide second order accuracy for concentrations and fluxes, including in the case of nonlinear isotherms.

The boundary conditions enable lattice Boltzmann simulations of solute transport in porous media with adsorption or reactions taking place on the material surfaces. The accuracy and second order convergence have been validated both theoretically and numerically. Some applications will also be shown.

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Mathematical model of two-phase compositional flow in porous media in environmental applications

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This work deals with two phase compositional flow. We present equations describing two phase flow, component transport and interphase mass transfer. For this type of problems, we propose a numerical method based on the mixed hybrid finite element method. We implement several variations of this method using different approaches to solving resulting system of linear algebraic equations. We use direct and iterative solvers and parallel implementation using MPI. The method is verified on problems for which exact solutions are known or solutions can be found in literature. Numerical experiments show that the errors are similar for all variations of the method. The method is convergent and the order of convergence is slightly less than one. There are significant differences in the computational time. Iterative solvers are faster and the parallelism is advantageous while using fine meshes. In the next part, we focus on the compositional flow. Data from two experiments are used and numerical results are compared with measured values. The first experiment was focused on evaporation of dissolved TCE. For low air flow rates above the water table, there is a good match with experimental data. For higher flow rates, the results differs. The second, more complex experiment in larger scale examined the influence of water table fluctuation and rainfall events on evaporation and transport of the dissolved TCE. For water table fluctuation, there is a good match with experimental data but for rainfall events there are significant differences. During the rainfall events there are uncertainties concerning the experimental data. Differences between the measured values and the numerical simulations indicate certain limits of the mathematical model used or the influence of other processes that are neglected in the current model. Finally we focus on hypothetical scenarios of vapor intrusion. In the field scale, we examine effect of water table drop or rainfall events, that were in smaller scale studied experimentally. Numerical results are similar to the second experiment.

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On the late time behavior of a relaxation compositional flow problem modelling the injection of heated fluid in a porous media

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We are interested on the non-isothermal compositional flows in porous media driven by relaxation balance laws induced by reaction among the species in a flow and linked to a hyperbolic conservation laws in a equilibrium model or stratified variety supported by theory and numerics. For concreteness, we are primarily interested in analysing this situation for class of systems of conservation laws modeling the injection of heated fluid in a porous media. The non-equilibrium system is modelled by a system of conservation law equations with relaxation source terms. Such flow problems leads to a strong coupling between the fluxes and the source terms and are generally hard to solve. By means of a cheap predictor-corrector unsplitting finite volume scheme (conservative by construction) and by a novel Riemann solution analysis for such nontrivial model at hand, we study the asymptotic time behavior of (possible) global smooth solutions supported by underlying modelling of the flow equations. In particular, we were able to give a 4 x 4 example in which the relaxation solution and the equilibrium solution differ in the physical space, but the same solutions agree in the phase space. Numerical simulations are presented and discussed in order to support the design of the construction of the proposed method and also to show some evidence we are computing qualitatively correct approximations.

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Operator-Based Linearization for the robust subsurface simulation

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The nonlinear nature of flow and transport in porous media requires a linearization of governing equations for the numerical solution. The new linearization approach is applied in this work to complex thermal-compositional problems of practical interest. The key idea of the approach is a transformation of discretised mass and energy conservation equations to an operator form with separate space-dependent and state-dependent operators. This transformation provides an opportunity for an approximate representation of exact physics of a problem through the interpolation in physical parameter space. This becomes similar to an approximate representation of space and time discretization performed in conventional simulation. Maintaining control of the error in an approximate physics, we perform an adaptive coarsening to identify major nonlinearities in a physical description. This strategy was applied to challenging flow problems with various physical kernels including thermal-compositional and reactive transport. The proposed strategy improves the robustness and efficiency of the nonlinear solution. The proposed approach provides opportunities for generic construction of physics-based proxy models with a full control of approximation error and migration of a simulation code to emerging computational architectures.

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SEMI-CONTINUOUS THERMODYNAMICS THEORY FOR A MULTIPHASE & MULTICOMPONENT RESERVOIR SIMULATION FRAMEWORK.

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Multiphase and multicomponent mixture flow are present in a several spectrum of applications, which goes from industrial process improvement to oil extraction. Modeling a multiphase and multicomponent flow usually involves volume-averaged procedure in N and M discrete phases and components, respectively. Unfortunately, in some applications, this modeling technique can be computational intractable, e.g., oil extraction, due to the large number of compounds needed to better represent the phenomenon of interest. In order to overcome this, most of multicomponent can be represented by a probability density function (PDF) and others some compounds can be still described by a discrete framework, Jatoba et al. [2014], Laurent et al.[2009], Lage [2007]. This approach, called semi-continuous thermodynamics (SCT) Cotterman et al. [1985], is often used to reduce the computacional cost of simulation with a large number of compounds. Likewise, this present work reformulates the conservation laws in porous media using SCT theory. The numerical validation is performed by comparing the classical discrete and the SCT approaches on 1D cases. Then, this methodology is extended to a simple 3D simulation case.

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A fractal graph model of capillary type systems

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The capillary system is modeled by a fractal graph attached to a blood vessel. It is supplied with differential equations obtained from three-dimensional model by the dimension-reduction procedure. The geometry and physical parameters of this system are described by a finite number of scaling parameters which allows for system to have self-reproducing solutions, solutions which are determined by their values on a certain finite piece of the fractal graph and are continued on the remaining part by using these scaling factors. We describe all self-reproducing solutions and, as a result we obtain a connection between the pressure and the flux at the junction point between the capillary system and blood vessel. This connection gives an artificial boundary condition at the junction in the blood vessel and allows to solve the problem for the flow in the blood vessel without solving it in the capillary system.

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Adsorption Stress and Deformation of Nanoporous Solids

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Experimental demonstration of adsorption-induced deformation of microporous adsorbents has been known for a long time, starting from the pioneering work of Meehan in 1927 on charcoal swelling upon CO2 adsorption. Later, it was shown with multiple examples that guest molecules adsorbed in pores exert a significant stress in the host solid matrix causing, depending on the conditions, not only swelling but also contraction, and sometimes matrix structural transformation and even collapse. With the advent of metal-organic frameworks, the adsorption deformation has attracted renewed attention due to the enigmatic phenomena of gate opening and breathing. Adsorption deformation has important implications and potential for the development of high-performance adsorbents and drug delivery vehicles. It takes place in geological formations, like micro-mesoporous domains in shale and coal reservoirs, where the deformation induced by CO2-methane displacement may cause significant reduction of permeability and even affect the mechanical integrity of reservoirs. I will present a general thermodynamic approach to predicting adsorption-induced deformation in nanoporous materials based on the notion of the adsorption stress. The adsorption stress is defined as the derivative of the grand thermodynamic potential of the adsorbed phase with respect to the variation of the sample strain. It can be calculated based on adopted adsorbate-adsorbent models from the classical density functional theory or Monte Carlo atomistic simulations. The adsorption stress introduced into the linear poroelasticity theory provides a unified framework for extension of classical poromechanics to nanoporous materials. Special attention will be paid to the specifics of adsorption deformation in micropores of molecular dimensions and the interpretation of the strain measurements in situ XRD and dilatometry experiments. I will show how the adsorption strain isotherms can be employed for evaluation of the micropore size distribution. Examples include micro- and mesoporous carbons and MOFs.

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An improved KJS method for analysis of dual pore size distributions in natural heterogeneous porous materials

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The conventional calculation methods of pore size distribution (PSD) are based on the simplistic assumption of single-pore-type. These methods may give inaccurate results when we deal with some heterogeneous porous materials. For example, since the mesopore structure of shale is irregular and various in shape, some widely used models like BJH method[1] and KJS method[2] will probably misinterpret the PSD by assuming a simple cylindrical pore geometry[3]. We present an improved KJS method by utilizing both adsorption and desorption branches of nitrogen isotherms and deriving the volume distributions of both cylindrical pores and slit pores. Condensation occurs in capillary pores when the relative pressure reaches a critical value corresponding to the Kelvin radius r_k. Besides that, the KJS method corrected the form of Kelvin equation to provide a better representation of the experimental relation between the pore size and the relative pressure of capillary condensation. Note that the pores in natural porous materials (like clay, coal, and shale), however, unlike the synthetic material, are heterogeneous, so they cannot be simply assumed as cylindrical pores. We suppose the pores in natural materials are either in cylindrical-shape or in slit-shape, or in a shape that can be interpreted as the combination of both of them proportionally. Based on the above assumptions of dual pore types, we revise the KJS-extended Kelvin equation as Eq.1, where p_m is saturation pressure of the adsorptive, the surface tension γ=8.85×〖10〗^(-3) N/m when gas is at the liquid-nitrogen temperature T=77.3 K, the molar volume of the condensed liquid v_m=34.677 〖cm〗^3/mol when liquid nitrogen is at equilibrium, R is the universal gas constant, and r_c and w_s are true radius/width of cylindrical pores and slit pores considering adsorption film thickness. Following a similar derivation like BJH method, by use of both adsorption and desorption isotherms, the basic equations are derived (see Eq. 2), where x=p/p_m is relative pressure, and v_a (x) and v_d (x) are the changes of absorbed quantity in a certain range of relative pressure during adsorption and desorption, r_k (x), r_k'(x) and t(x) are the Kelvin radius of cylindrical pores and slit pores and the adsorption film thickness, V_c (x) and V_s (x) are the distribution functions of cylindrical pore volume and slit pore volume. And after applying mean value theorem and dividing the intervals upon Eq. 2, we can obtain the formula of calculating PSDs. The whole implementing procedure can refer to Fig. 1. Eventually, the presented method is applied to analyze the pore structure characterization of shale sample. The results depict that both the adsorbed quantities and PSDs can be separated into two distinct parts contributed by cylindrical pores and slit pores respectively (see Fig. 2). In other words, the proposed method in this paper can distinguish clearly between the two types of pores. It provides us a better understanding of the complicated pore structure of shale-like natural heterogeneous porous materials.

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Behavior of water in partly nanoporous biopolymer composites

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Transport phenomena and material behavior of porous biopolymer composites like wood are mainly influenced by the water sorption and the chemical structure of the material. Information in this field provides possibilities for a better usage of lignocellulosic materials in classical construction, actual modification and high advanced products.

The structure of such biopolymer composites like wood is not understood completely yet. Circum-stances in different analytical fields are caused by the absence or the presence of water. Especially bound water which does not freeze but is reasonable for the swelling and shrinking of the material is one main problem. Actual theories indicate a tightly bound interaction of the water to the OH-groups of the material as main reason for the behavior of this water type.

Wood is a mainly meso- and macroporous material. The presence of micropores is shown too in newer publications. These existing nanopores, caused by the structure of the biopolymer could be influence the water state and the non-freezing behavior too. The main question is how to investigate these types of pores in organic materials and distinguish between the different bonds of water.

In general a leak in mathematical modelling of this topic in wood science is determined. Additionally the analytical techniques have to be improved to investigate lignocellulosic materials which are sen-sitive to high temperatures.

The presentation will focus on past and actual research results regarding the understanding of the porous structures of wood and bound water as well as own actual research in this field. These investigations are going on to explain the relationship between the change of mechanical properties at different moisture contents and the chemical structure of the materials. This is done by studying the thermodynamically behavior and the porosity of the materials with different experimental methods compared to mechanical testing.

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Capillary Condensation in Disordered Mesopores

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The traditional models used to analyze adsorption and capillary condensation in mesoporous materials assume geometrically ideal pore shapes, such as cylinders. Although these models go back to the nineteenth century and the work of Lord Kelvin, it is only relatively recently that one could produce materials with the same pore geometry as assumed in the models, and thereby to test them rigorously [e.g. 1]. These experimental works have raised fascinating questions about the impact of geometrical disorder on adsorption and capillary condensation, and they have triggered a series of theoretical researches. Many recent works have investigated the role of mild elements of disorder, such as local constriction or corrugation superimposed to otherwise geometrically ideal cylindrical pores [2,3]. However, the relevance of these perturbation-like results to fundamentally disordered materials, such as most materials of practical interest, is unclear.

In the present communication, we use a probabilistic model to investigate adsorption and capillary condensation in truly disordered mesoporous solids. We generalize the Gaussian-random-field models of porous materials [4] so as to describe the structure of both the porous material and of the liquid condensate (Cf. Figure). This modeling approach enables one to analyze the free energy landscape of the condensate in very disordered solids using a low-dimensional configuration space. We illustrate our modeling methodology with the case of nitrogen adsorption in carbon xerogels; we notably show that the generalized Gaussian-random-field approach enables one to predict the adsorption isotherm starting from the small-angle scattering characterization of the material.

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Chiral Phases of a Confined Cholesteric Liquid Crystal: Anchoring-Dependent Helical and Smectic Self-Assembly in Nanopores

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Chiral liquid crystals (ChLCs) allow a fundamental insight into the interplay of molecular chirality and the formation of macroscopic, self-assembled helices. They also exhibit unique optical properties, in particular huge polarization rotation, which is employed in a wide range of photonic technologies. Here, we present a study of linear and circular optical birefringence in combination with X-ray diffraction experiments on an archetypical ChLC, i.e., the cholesteric ester CE6, confined in cylinders of mesoporous alumina and silica with distinct polymer surface graftings resulting in normal or tangential wall anchoring. The unconfined ChLC exhibits a discontinuous, first-order isotropic-to-chiral nematic (cholesteric) phase transition with the formation of double-twist helices and a discontinuous cholesteric-to-smectic A transition. The thermotropic behavior of the confined ChLC, explored in a channel radii range of 7–21 nm, deviates substantially from bulk behavior. There is no isotropic state. In contrast, a chiral paranematic phase with a preferred arrangement of the ChLC at the channel wall is found. For normal anchoring, a radial-escape structure evolves upon cooling. The phase transition to the smectic phase is completely suppressed. For tangential anchoring, a large optical activity indicates a continuous paranematic-to-cholesteric transition with double-twist helices aligned parallel to the long axes of the cylinders. Upon cooling, these helical structures, known as basic building blocks of blue ChLC phases, transform in a continuous manner to a cylinder-aligned smectic A phase. [1]

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Comprehensive characterization of disordered nanoporous materials combining gas physisorption with scattering methods

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Since the discovery of the M41S mesoporous silicas, the design of novel nanoporous materials evolved very fast providing systems with improved catalysis, sensing or separation properties. However, the material characterization, with special regards to porosity, became much more challenging due to the higher complexity of these systems. Standard characterization methods, e.g. gas physisorption, are in many cases not enough for clear understanding of porosity features and therefore more advanced approaches are required. One possible solution is the combination of gas physisorption with small-angle scattering of X-ray or neutrons. The so called in situ SAXS/SANS-Physisorption experiment revealed to be an useful and elegant method especially for the investigation of structures with complex disordered pore networks. In principle, during the adsorption of specific adsorptives, which have the same electron density as the material matrix, only the void pores will contribute to the X-ray/neutron scattering. In this way, the pore filling process can be precisely monitored and the accessibility of the porous network determined. Moreover, the porous properties of the system (e.g. free surface area and pore sizes) can be independently obtained by the SAXS/SANS curves at different filling grades applying case related analysis approaches. In this paper, different applications of the in situ SAXS/SANS-phyisisorption experiment will be presented. These case studies will deal with the porosity investigation of materials of different nature such as porous silica, organosilica and carbon.

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Coupling behavior between adsorption and deformation of nanoporous materials: a multiscale study

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Adsorption-induced deformation is a ubiquitous phenomenon observed in various nanoporous materials. This coupling of adsorption and deformation involves both the solid-fluid interaction at the molecular level and the interaction between neighboring domains at the mesoscale. We present a multiscale framework to model this behavior by employing molecular simulation, thermodynamics and Dependent Domain theory [1] at different scales. Hybrid Grand Canonical Monte Carlo (GCMC)/ Molecular Dynamics (MD) simulations are carried out at microscale to study the solid-fluid interaction in individual cylindrical nanopores of different sizes, from which both the adsorption and deformation isotherms are acquired. The simulation results show that the adsorption process is initiated by a thin film stage, followed by an abrupt jump to a filled pore and ending with the flattening of the pore meniscus. Each stage corresponds to a distinct deformation behavior: shrinkage in the thin film stage and swelling in the final stage after the capillary condensation (Figure 1). Further analysis shows that the shrinkage is caused by the compressive surface stress at the solid-fluid interface while the swelling is attributed to the change of the Laplace pressure at the liquid-gas interface as the meniscus is flattening. Fluid configuration hysteresis is observed, between adsorption and desorption for chemical potential near the condensation point, which results in mechanical hysteresis. In addition, a series of simulations are carried out to study the influence of pore size, Young's modulus and wetting energy on the sorption and deformation behavior at microscale. A thermodynamic model is then proposed to classify the results of molecular simulation. By considering the thin film and filled pore stages separately, this model gives a good description of our molecular simulation results and identifies the contribution of surface stress, disjoining pressure and Laplace pressure to the deformation of the nanopores at different stages. Taking the thermodynamic model as a bridge, we upscale the results from the molecular simulation to a mesoscale porous system containing a collection of nanopores, with different pore radii, embedded in a solid matrix. The adsorption and deformation behavior of the porous systems is then described by the Dependent Domain theory, taking into account both the occurrence of percolation and the mechanical interactions between neighboring pores. We calculate sorption and deformation isotherms including scanning curves and subloops and find that systems may exhibit significant dependent domain effects due to the neighboring pore interactions (Figure 2), which could not be captured by the classical Independent Domain theory [2]. Further, a series of simulations is conducted to study the influence of geometrical factors including pore arrangement and pore size distribution.

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Coupling Between Hydrocarbons Recovery and Elastic Relaxation Inside Kerogen's Nanoporosity

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Shale-gas recovery from unconventional reservoirs is a very slow process that exhibits anomalous behavior at large scales such as non-Fickian productivity decline. Important work, focusing on the subnanoporosity of the organic matter called kerogen (where the hydrocarbons are produced and trapped during maturation), has been recently carried out to elucidate these features [1,2,3]. Unfortunately, the molecular force field needed to construct the kerogen replicas used in these studies is not adapted to capture flexibility effects such as swelling upon fluid adsorption. Even if certainly limited in the case of mature kerogens, we believe that flexibility effects can be important to the understanding of hydrocarbon transport in kerogens. In this work we present a re-parameterization of the non-bonded part of the AIREBO C/H potential, achieved to reproduce experimental equations of state for alkane chains, and use it to study the mechanical properties of two - raw and fluid-filled - porous amorphous carbon matrices obtained from quench molecular dynamics simulations, serving as proxies for mature and immature kerogens. While, as expected, the mature matrix is somehow insensitive to pressure and temperature effects, we observe a huge dependence of the density (and thus porosity) of the immature matrix on applied pressure, temperature and fluid loading. Especially, while some open porosity might be observed at atmospheric pressure, the raw immature matrix significantly shrinks in volume at geological pressures (25-100 MPa) where only traces of closed porosity remains. However, the presence of trapped/adsorbed hydrocarbons can significantly open the porosity. Finally, we analyze the interplay between hydrocarbons recovery and elastic relaxation. We believe that this strong coupling leads to anomalous behaviors, intrinsic to kerogens nano-porosity, which could give a decisive understanding of the shale-gas recovery process.

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Defect topologies in chiral liquid crystals confined to mesoscopic channels

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Soft matter confined to volumes of nanoscopic extent constitutes an interesting class of systems. In particular a lot of work has already been invested to study confined liquid crystals. The focus of this study is the orientational order of liquid-crystals and especially their deformation. In the case of non-chiral nematic liquid crystals one immediately may think of the twisted-nematic cell where the nematic director rotates between the substrates and a quasi-cholesteric helix evolves. The more recent research focuses on confined chiral phases, e.g. cholesteric or blue phases. If the introduced substrates are separated by a distance which is not equal to a multiple of half pitches transitions between the inherent defects of blue phases may be observed. Two-dimensional confinement (i.e., circular or rectangular mesochannels) of liquid crystals has been less far studied to date. In the late 1970s and early 1980s theoretical studies focused on the orientational order of nematic phases in tubular spaces. However, to the best of our knowledge there is no systematic study of chiral phases confined in two dimensions up to date. In our study we focus on two-dimensional confinement of chiral liquid crystals where we observe a host of novel topological defects. Furthermore, the geometry of the chosen channel and its surface anchoring determines the defect structure.

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Density Functional Predictions for Sorption Isotherms and Drying Shrinkage of Multi-Scale Porous Structures

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The adsorption/desorption isotherms in porous media is a powerful and widely-adopted method to probe the pore size distribution and connectivity of the pore network. Despite the importance of the isotherms, the picture of capillary condensation in a single infinitely long pore of simple geometries (slit, cylinder, etc.) and the corresponding hysteresis loop is not capable of describing the experimental results which are measured in highly connected, irregularly shaped and three dimensional pore networks. Based on the classical density functional theory, we developed a parallelized numerical scheme to model the adsoprtion/desorption processes in these multi-scale porous structures with different adsorbate/adsorbent pairs. Our only parameters, the fluid-fluid and fluid-solid interactions are calibrated by adsorbate critical point, surface tension, and molecular adsorption simulations. Given porous structures from either meso-scale modeling or TEM photography, we for the first time predict the adsorption/desorption isotherms and calculate specific surface areas for a variety of multi-scale porous materials and adsorbates which are in good agreement with experimental results. We use these ab initio calculations to demonstrate and discuss several different mechanisms for hysteresis. Furthermore we produce the three dimensional distribution of adsorbed liquids inside the pore network and calculate local capillary stresses, to discuss the role of capillary pressures in mechanical properties of cement and investigate the drying shrinkage phenomena.

Figure 1: A simulated nitrogen adsorption/desorption curve on a meso-scale colloidal model of cement structure. Adsorption part is in very good agreement with experiments, while in the desorption part the colloidal model intrinsically presents much larger connectivity of pores therefor very few bottleneck effects and much less hysteresis.

Figure 2: A simulated water adsorption/desorption curve on the meso-scale colloidal model of cement structure. Same lack of bottleneck structures leading to less hysteresis as in the nitrogen case.

Figure 3: Snapshots of a cross-section during water adsorption/desorption, showing the 2d projections of 3d real capillary miniscus and some bottleneck effects.

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Effect of pore geometry on the compressibility of confined simple fluids

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Compressibility of a fluid is its fundamental thermodynamic property, which can be experimentally determined from the sound velocity. Ultrasonic experiments on fluid-saturated porous materials allow obtaining information on the compressibility of the fluids confined in the nanopores (1-2). The results of these experiments suggest that similarly to many other thermodynamic properties, compressibility of a confined fluid differs from compressibility of a bulk one at the same conditions. This is confirmed by Monte Carlo molecular simulations in the grand canonical ensemble (3-4), which allow calculation of the compressibility from the fluctuation of number of particles in the system (5). Motivated by experiments from Ref. 2, the calculations were performed for a simple model system: Lennard-Jones argon in spherical silica pores (3-4). These methods have been shown to be quite accurate for pores 2.5 nm and larger, but have difficulties for smaller pores. Spherical pore below ca. 2 nm can accommodate less than 100 molecules. Below this number, the fluctuations become non-Gaussian, making compressibility calculations inapplicable. However, a model of long cylindrical pore can resolve this problem: while the pore diameter can secure substantial confinement, the length provides a sufficient number of molecules in the system. In this work, we generalize the model from Ref. 3 to cylindrical pore model. This allows us to perform the calculation of compressibility for pores below 2.5nm diameter and also to find how much the pore geometry affects the compressibility. We found that compressibility of argon in cylindrical pores larger ca. 2.5 nm do not differ qualitatively from the spherical pore results: giving the same relationship between the compressibility and pore size as for spherical pores (4). Interestingly, the results of the calculations for smaller pores showed that this regularity breaks below 2.5 nm even when the fluctuations are Gaussian. That confirms the well-known distinction between micro- (less than 2 nm) and meso- (larger than 2 nm) pores. Note that the theoretical predictions of the compressibility of a confined fluid not only shed light on the fundamental understanding of confined systems, but can also provide valuable information for predictions of flow properties of fluids in nanoporous media, e.g. hydrocarbons in shale gas (6).

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Elastic properties of fluids adsorbed in nanopores

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Ultrasonic measurements are a versatile tool for the study of materials adsorbed in porous media providing an insight into a multitude of properties. For example, sorption-experiments with various materials (argon, nitrogen, oxygen and alkanes) in Vycor glass reflect both the spatial distribution of the adsorbates as well as a continuous solidification in a broad range of temperatures (see, e.g., [1]). Depending on the adsorbate and its interactions the elastic properties of the surface layers can differ considerably from those of the capillary condensate. In addition, ultrasonic studies allow us to determine some fundamental quantities related to sorption-induced deformation: the adsorbate exerts a normal pressure on the porous matrix that in turn has an impact on its own properties. The linear pressure dependence of the adsorbates' longitudinal modulus allows us to deduce the normal pressure at saturation as well as the corresponding change of surface stress [2,3]. We shall present an overview of experimental results and unsolved problems.

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Elasticity of Fluid in Solvophilic and Solvophobic Confinement

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The velocity of ultrasonic waves in fluid-saturated porous media is a function of elastic moduli of solid and fluid constituents [1,2]. Therefore, when the properties of a solid are known, ultrasonic measurements can provide information on the bulk modulus of the fluid in the pores. Ultrasonic experiments on fluid-saturated nanoporous glasses suggested that the bulk modulus of fluids in the pores is affected by confinement [3,4]. Recently Schappert and Pelster measured the velocity of ultrasound propagation in nanoporous Vycor glass saturated with liquid argon and determined the modulus of confined argon from those measurements [4]. The simplicity of argon allows one to model this system on molecular level and make a quantitative comparison of the model predictions and experimental results. Here we present the results of calculations of bulk modulus of liquid-like argon in spherical silica pores carried out using two different methods. First, the modulus is derived from the average fluid density [5], where the density is predicted using the density functional theory method [6]. The second method is based on Monte Carlo simulations in the grand canonical ensemble, the modulus in this case is calculated from the fluctuations of the number of molecules in the system [7]. We show that the predictions of the two methods are consistent and close to the modulus derived from the ultrasonic experiments [4]. Varying the pore size we show that the modulus of confined liquid argon linearly increases as a function of the reciprocal pore size; for example, the modulus of argon confined in a 2.5 nm pore exceeds the modulus of bulk liquid argon by a factor of two. Additionally, we vary the solid-fluid interaction parameters to represent solids other than silica and find how it affects the fluid modulus. We show that weaker solid-fluid interactions, which are yet solvophilic, still cause the increase of the fluid modulus, but this increase is less pronounced. However, if the solid-fluid interactions are weaker than the fluid-fluid interactions (solvophobic confinement), the opposite effect is observed: fluid in solvophobic confinement has lower modulus than the bulk fluid. Therefore, we conclude that nanoconfinement alters the fluid modulus. However, it is not the confinement per se which changes the fluid modulus, but the solid-fluid interactions. Solvophilic confinement makes the fluid stiffer, while solvophobic confinement makes it softer. These effects have to be taken into account when considering wave propagation or fluid flow in nanoporous media.

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Freezing and Melting of Aqueous Salt Systems in Nanopores

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Phase transitions in nanoscale confinement are fundamentally different from those occurring in bulk. For pure substances these differences have been studied in some detail, but little attention has been paid to mixtures. We study solid/liquid phase transitions of aqueous alkali halide systems in the pores of MCM-41 and SBA-15 mesoporous silica by calorimetry and X-ray diffraction. DSC cooling/heating scans are performed to map the freezing/melting phase diagram of aqueous salt systems in the pores with or without external excess phase. We have found [1] that the confinement-induced shift of the eutectic temperature of aqueous alkali halide systems in nanopores can be significantly greater than the shift in the melting point of pure water. Greatest shifts are found for salts that crystallize in form of oligohydrates at the eutectic point. This can be explained by the larger fraction of pore volume occupied by salt hydrates as compared to anhydrous salts, on the assumption that precipitated salt constitutes an additional confinement for ice/water in the pores. In-situ small-angle x-ray diffraction was used to determine freezing/melting-induced deformations of the pore lattice of SBA-15 and MCM-41, as described for pure ice/water by Erko et al. [2]. For eutectic solutions of several salts we obtain lattice strain vs. temperature scans with three distinct regions, as in the case of ice/water: Starting from the solid eutectic mixture at low temperature, the formation of a liquid-like layer at the pore walls leads to lattice expansion (region I), eutectic melting in the pore in the presence of external solid causes an abrupt contraction (region II), followed by a nearly linear lattice expansion up to the temperature at which the external phase melts (region III). Interestingly, this behavior is modified for salts exhibiting a phase transition in the solid state, such as in the case of NaBr.

Figure 1. (a) DSC heating scans for eutectic salt systems in SBA-15 normalized to the bulk eutectic temperature (TE); (b) Pore lattice strains monitored by the position of the 10 Bragg peak as a function of temperature for eutectic aqueous NaCl system in SBA-15.

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Freezing temperatures and solubilities in confined electrolyte solutions

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Crystallization of solid phases in pores is a major cause of damage in building materials. The underlying solid–liquid equilibria are strongly affected by pore size. For example, it is well known that there is a significant reduction of the freezing temperature of ice with decreasing pore size (e.g. [1]). Similarly, it is known that there is a strong solubility increase of salts with decreasing pore size due to the limited crystal size in nanopores [2]. In effect, the phase diagrams of binary systems such as aqueous electrolyte solutions are significantly altered under conditions of confinement in mesoporous materials. In this contribution we will report on a thermodynamic modeling study of the influence of pore size on the solid–liquid equilibria in electrolyte–water systems. The model is based on an analysis of the influence of crystal size on the chemical potential of both ice and salt crystals. However, the calculation of the freezing temperatures of water also considers the additional influence of the dissolved electrolytes on the freezing point depression. Finally, the solubility increase of small crystals is calculated and the complete phase diagram is constructed. A significant shift of the cryohydric point to low temperatures is predicted, i.e. the lowest temperature at which a liquid solution can still exist under equilibrium conditions. We also report on an experimental determination of freezing temperatures in binary electrolyte systems (e.g. KCl–H2O, NaNO3–H2O, KNO3–H2O) using a calorimetric technique. In these measurements the depression of the cryohydric points to lower temperatures is confirmed which agrees with both previous experimental studies [3,4] and the model predictions. A comparison of calculated and experimental freezing temperatures will be provided.

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Hydrocarbon storage mechanism in shale reservoirs and impact on hydrocarbon production

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This paper summarizes the results of an experimental study designed to investigate the mechanisms of hydrocarbon storage in shale reservoirs and their impacts on the production of hydrocarbon. The experiments consisted in measuring the total NMR amplitude associated with Barnett and Eagle Ford shale samples saturated with methane and ethane at different level of effective stress. During our measurements, the pore pressure was incrementally raised and reduced between 300 psi and 4000 psi. The confining pressure and temperature were kept constant at 5000 psi and 30°C, respectively. Methane was used to understand the storage mechanisms in the dry gas window while ethane was used to study the storage mechanisms in the oil window because it goes through a phase transition from gas to liquid at a pressure of 675 psi at 30°C. The measurements with methane show that gas compressibility is the main storage mechanism at pore pressures larger than 2000 psi in the dry gas window. At pore pressures lower than 2000 psi, adsorption becomes important as the pore pressure decreases. Adsorption allows the storage of more than twice the amount of gas that would be stored without adsorption. The measurements with ethane show that liquid compressibility controls the storage of hydrocarbon at pressures greater than the bubble point, in the oil window. Below the bubble point, capillary condensation can increase the storage capacity of shales by more than a factor of 8. The pore pressure depletion experiments show at effective pressures greater than 3500 psi, a pore space reduction by as much as 23% in some samples, because of pore compressibility. In the dry gas window, the absorbed gas and the free gas are produced simultaneously until a pore pressure of 2000 psi. Below 2000 psi, adsorption hinders the production of gas. In the oil window, capillary condensation reduces the amount of hydrocarbon producible below the bubble point.

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Hydrodynamic finite-size effects on diffusion under extreme confinement.

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Fluids transport through nanoporous media is a key issue for unconventional hydrocarbons recovery or for cap rock integrity in the context of CO2 sequestration. The thermodynamic behavior of a fluid in a clay nanopore depends on the nature of the clay itself and on the physico-chemical effects induced by the confinement. Most studies on the hydrodynamics of confined fluids on the molecular scale are based on model systems such as a Lennard-Jones (LJ) fluid between LJ walls, though some applications to more realistic systems have been published, as water in silica nanopores [1] or between two montmorillonite layers [2,3]. Such molecular dynamics (MD) simulations are necessary in the contexts previously described to make the transition from molecular descriptions to continuous ones in order to upscale transport properties from the microscopic to the macroscopic scale.

It is well established that MD calculations of some transport coefficients, such as the diffusion coefficient, can suffer some finite-size artefacts arising from hydrodynamic effects [4]. We recently demonstrated that the shape of the simulation box (anisotropy), that has been ignored so far, also plays an important role [5]. A confined system is by definition anisotropic: In a slit pore, both the physically relevant confining distance and the simulation-required finite lengths in the directions along the surfaces may influence the result. Here we discuss the finite-size effects in surface-parallel directions for model systems (LJ). We analyze these effects in the framework of continuum hydrodynamics. We demonstrate that this hydrodynamic contribution to the diffusion coefficient explains most of the molecular simulation results. In turn, this allows us to correct the simulation results for finite-size effects in the (non-physical) box size along the surfaces, thereby allowing to disentangle the dependence on the physical confining distance between the surfaces.

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Hygromechanical behavior of biopolymeric nano-composite material: from MD simulations to poromechanics

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In presence of water, biopolymers of vegetal origins show a rearrangement of their internal structure, influencing their physical properties. The swelling of the wood cell wall S2 layer, a nanoporous composite material that interacts strongly with moisture, is such an example. To understand this hygromechanical behavior, we use an upscaling from molecular dynamics simulations (MD) at the atomistic scale to a poroelastic model, which is implemented in finite-element modeling (FEM) at the cell wall scale. Using an atomistic approach (molecular dynamics MD), we study different components: cellulose, galactoglucomannan, xylan, lignin, a cellulose microfibril and a microfibril aggregate. The coupled effects of water sorption on hygric and mechanical properties are investigated. The model is studied with MD simulations, where the explicitly present atoms are moved by integration of the Newton equation of motion. The MD models have size of a few nanometers or several thousands of atoms and are put in full periodic boundary conditions. A typical time scale of a simulation is 10 ns with time step of 1 fs. First, we study the hygrothermal behavior of the pure polymers at the lower scale. During adsorption, water molecules are seen to first fill the existing pore space and afterwards displace the polymeric chains, leading to a nonlinear swelling and a weakening of the mechanical properties, due to changes in the hydrogen bond network and the presence of adsorbed water layers in the polymers at high moisture content. As a result, the stiffness, particularly in shear, decreases non-linearly, which is explained by breaking of numerous hydrogen bonds due of sorption. Further, still using Molecular Dynamics (MD) simulations, we constructed and investigated models of cellulose microfibrils and aggregates, that consists of crystalline cellulose, amorphous hemicellulose and lignin. Water molecules are adsorbed in the amorphous hemicellulose, but also excess of sorption on the interface behavior to components is observed. No sorption occurs in crystalline cellulose. The existence of two different regions in moisture response is demonstrated. As the moisture content increases, water molecules are adsorbed in the bulk amorphous phase, but also preferentially at the interface, leading to a swelling that is proportional to the porosity increase and to a mechanical weakening. Based on the MD results, a nonlinear poroelastic model based on chemical potential and molar concentration as fluid state variables is developed to describe these fluid-related nonlinear phenomena. A thermodynamic consistent framework is based on a mixed higher order formulation of the energy function, accounting for nonlinear mechanical, fluid and fluid-solid coupling contributions. The formulation includes nonlinear effects like mechanical weakening and mechano-sorptive behavior, where mechanical stress influences the adsorption behavior. The poroelastic properties, like stiffness, moisture capacity and coupling coefficient, are determined from the MD simulations and are found to be function both of fluid concentration and mechanical stress. The coupling coefficient is found to equal the swelling coefficient and its dependence on stress and concentration is interpreted with respect to porosity change and

solid matrix deformation.

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Impact of temperature on the sorption-induced deformation of nanoporous glass

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We investigate the influence of temperature on the sorption-induced deformation of nanoporous glass [1]. Our study shows that small temperature changes can temporarily cause strong deformations of the porous material that decay in long time intervals of up to 1 week. This effect is probably related to the formation of vapor voids and the slow migration of the adsorbate within the pores. We expect that our observations for the model system of argon and porous glass can be generalized to other systems. Also in technical applications, such significant influences on the deformation in consequence of seemingly insignificant temperature changes should be taken into consideration.

Furthermore, during cooling we observe a continuous reduction of the expansion of the porous glass matrix caused by the adsorbed argon. The contraction is attended by a likewise continuous change of the adsorbed argon's phase state from liquid to solid. This simultaneous behavior evidences that the liquid–solid phase transition leads to a reduction of the pressure the adsorbate exerts on the pore walls.

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Influence of strained graphitic nano-pores on fluid transports: a Molecular Dynamics study with water, carbon dioxide and methane

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The study of transport properties in porous media plays an important role in many applications such as soil mechanics, geohydrology and the storage of nuclear waste. Along with the development of unconventional reservoirs (shale gas) extraction technology, like hydraulic fracturing, more attention has been paid to the transport of liquid molecules in carbon pores. Graphite, the most common form of solid carbon can be found in profound coal bed, under large compressive stress states, will be subject to the present study.

The modeling based on the Navier-Stokes equation, Darcy's law and the non-slip condition is usually used in the practice of engineering. However, when the fluid penetrates in nano graphite pores, both experiences and simulation results show that the fluid flux is underestimated by conventional no-slip condition. The Molecular Dynamics (MD) method is currently the best method for studying fluid-solid interfaces properties. The most MD simulations focus on the pristine graphite (graphene) or Carbon Nanotubes (CNTs). Meanwhile, graphite can be subject to mechanical strain due to different reasons, for example, both electromechanical force or high stress environment in mine can cause isotropic or anisotropic strain to the graphite surface. The surface strain can affect the fluid-solid friction and thus affect the permeability of graphite porous media.

In this study, using equilibrium molecular dynamic simulations and Green-Kubo formulism, we study the strain effect to the fluid-graphite surface friction and determine the slip length. Three common molecules in petroleum industry: water (H_2O, triangular shape), carbon dioxide (CO_2, rod like shape) and methane (CH_4, spherical particle) are considered in the simulations. From the simulations, we obtained fluid molecules structure and density information strongly correlated with slip length which is anisotropic in the most general case. A theory is also developed to provide an explanation for the strain-friction mechanism.

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Insights into the Adsorption and Phase Behaviour of Fluids in Nanoporous Materials with Hierarchical Pore Structure: Towards an Advanced Structural Characterization

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Recently, much effort has been devoted to the development of materials which exhibit hierarchical pore structure with the appropriate balance of micro- and mesopores, as well as advantageous pore connectivity. The network of interconnected micro- and mesopores facilitates efficient transfer of fluids to and from catalytically active sites, leading to benefits in numerous catalytic applications. A large amount of work has been dedicated to their pore structural characterization [e.g. 1], for instance by physical adsorption. Detailed insights into the pore architecture (pore size distribution, pore volume, and pore interconnectivity) are important because they control transport phenomena, diffusional rates, and govern selectivity. Gas adsorption is well suited for this characterization because it assesses a wide range of pore sizes, spanning the entire micro- and mesopore range. Within the last two decades major progress has been achieved in understanding the adsorption and phase behavior of fluids in ordered nanoporous materials and in the development of advanced approaches based on statistical mechanics such as molecular simulation and density functional theory (DFT) of inhomogeneous fluids (see reviews [1,2] and references therein). This progress, coupled with the availability of high resolution experimental procedures for the adsorption of various subcritical fluids, has led to major advances in the structural characterization by physical adsorption. These advances and corresponding recommendations for physisorption characterization are also summarized in the 2015 IUPAC technical report [2. However, for an in-depth characterization of the pore network (and the development of new methodologies), a detailed understanding of the adsorption and phase behavior of fluids confined in such complex pore structures is needed. This is crucial for advancing the application of nanoporous materials such as mesoporous zeolites in catalysis, separations. Within this framework we have investigated the adsorption and phase behavior of fluids such argon and carbon dioxide over a wide range of temperatures from below the triple point temperature up to supercritical temperatures in hierarchically structured micro-mesoporous zeolites and carbons. These unique data not only allow us to map details of the phase behavior (incl, pore condensation, hysteresis behavior), but also to advance methodologies for a reliable pore and pore network characterization of hierarchically structured nanoporous materials.

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Interaction of a Protein with Cationic Surfactants in Tubular Silica Nanopores

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The interaction of surfactants with adsorbed protein layers is of practical relevance in the context of surface cleaning and the removal of protein from porous separation membranes. We are studying the co-assembly of the globular protein lysozyme (Lyz) with the cationic surfactant cetylpyridinium chloride (CPC) in the tubular pores of SBA-15 silica (diameter 8 nm) using small-angle neutron scattering (SANS). Samples were prepared by equilibrating the matrix successively with solutions of the single components, starting either with protein or surfactant, and the amounts adsorbed (p and s) were determined by analysis of the supernatant solutions. SANS measurements of the slurry samples were made using a H2O/D2O solvent mixture that matches the scattering length density (SLD) of our SBA-15 silica. As the SLD of Lyz is similar to that of silica, the protein is not 'seen' by the neutron beam, but its influence of the assembly structures in the pores is detected indirectly by comparing SANS scattering profiles of samples with and without protein (Figure 1). The scattering profiles I(q) are modeled as described previously [1] as a sum of two independent terms: Bragg scattering from the pore lattice of SBA-15 (IBragg) and diffuse coherent scattering (Idiff) from surfactant/protein aggregates distributed in the matrix. IBragg(q) contains the form factor P(q) of the cylindrical pores that depends on the radially averaged scattering density profile in the pores and hence on the geometry of the surfactant/protein assembly in the pores. Results of this analysis will be presented and the implications for the interaction of the two components in the pores will be discussed.

Figure 1. SANS intensity profiles for different adsorption levels of protein (p) and surfactant (s) in SBA-15: Figure 1: Protein + surfactant in comparison to surfactant only, and influence of which component is pre-adsorbed; figure 2: Constant adsorption level of surfactant (s = 0.6) with increasing loadings with protein, and difference between true protein loading (p) and protein loading p0 that would have been attained in the absence of surfactant.

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Low-frequency dynamics of water confined in nanopores

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We show that Dynamical Mechanical Analysis (DMA) provides novel information on the low-frequency dynamics of water in nanopores. A distinct pore size dependence of the glass transition temperature of confined supercooled water is for the first time detected from a macroscopic mechanical experiment. In our experiments we use DMA with a frequency range of 0.2 – 100 Hz and investigate confined water in mesoporous Gelsil with pore sizes 2.6 nm and 5 nm and Vycor (10 nm pore size) in the temperature range 80 K – 300 K [1]. Analysis of thermal expansion data for different pore sizes indicates that the supercooled water is most probably arranged in a shell of maximal two layers, independently of the size of the pores. Thus, the observed pore size dependence of Tg cannot be a finite-size effect. The new physical picture that emerges then is that Tg depends on the mean curvature $\kappa \propto 1/d$ of the corresponding pore surface, which for zero curvature ($\kappa \propto 1/d = 0$) extrapolates to Tg(0) = 136 K, the traditional value of bulk water [2]. It is remarkable, that the glass freezing behaviour of such a small amount of one or two layers of water can be detected in a macroscopic mechanical experiment.

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Molecular orientation of a discotic liquid crystal in nanoporous solids

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Discotic liquid crystals (DLC) can exhibit a liquid crystalline phase with their molecules oriented along one specific direction forming hexagonally arranged columns. Embedded in nanoporous alumina or silica membranes the columns orient perpendicular (radially) or parallel (axially) with respect to the pore axis. Axially oriented columns ensure high conductivity in the stacking direction due to overlapping pi– electrons yielding interesting applications in e.g. organic semiconductor-based devices. We investigated the DLC 2,3,6,7,10,11 - hexakis [hexyloxy] triphenylene (HAT6) embedded in nanoporous alumina and silica membranes. Due to their hydrophilic nature porous membranes enforce face-on anchoring leading to a radial orientation. The orientational order of the liquid crystalline columns can be probed by optical birefringence measurements [1, 2]. By chemically changing the silica anchoring conditions from face-on to edge-on the HAT6 molecules still orient radially arranging into columns that follow the curvature of the pore surface. The distortion present due to the bending of the columns in the radial orientation is energetically more favorable than the lattice distortion present for an axial orientation. Interestingly, a quantized phase transition of each molecular layer is found indicated by a distinct increase of the optical orientation (Figure 1). Additionally, an axial orientation of HAT6 filled into alumina membranes with a diameter of 25 nm is achieved (Figure 2). We suspect that due to the long filling time at high temperatures and high volume-to-surface ratio anions introduced into the membrane lattice from the manufacturing process react with the DLCs changing the anchoring condition of the membrane. This enforces edge-on-orientation leading to an axial orientation of columns. X-ray diffraction (XRD) experiments giving detailed information about the translational order support the findings from optical measurements.

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Multifunctional bio-based porous materials for sustainable construction

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Some multi-scale building materials, like wood and hemp concrete or daub, exhibit high potential properties in terms of thermal and hygrometric diffusion (thermal insulation, moisture expelling out of a house). However, the correlation between these specific properties and the multi porous structure is complex and still unclear. In order to get a better insight into the precise origin of such multifunctional properties, new model systems based on polymeric materials with double porosity have been envisioned. Bi-porous polymer networks with controlled nano- (200 nm) and macro- (200 µm) pore sizes and connectivity have been designed and elaborated with the aim to investigate the role of each porosity level on their properties. As a reference system, we have initially prepared bi-porous poly(2-hydroxy methacrylate) (PHEMA) in which nanopores arise from the removal of a porogenic solvent (EtOH) and macropores are formed from particle leaching of fused or non-fused NaCl particles (Fig. 1 as an example) [1]. To obtain bio-based polymer systems, the synthesis of porous materials has been adapted with monomers derived from natural products, such as clove (eugenol), tannins (gallic acid), and catechins (epoxy network developed as Bisphenol A alternatives). The pore morphology (in particular, size and interconnectivity) has been analyzed by mercury intrusion porosimetry and SEM. The mechanical properties, thermal diffusion, and soaking/drying behaviour will then be studied (with new non-invasive methods for fluid transport, i.e. IRM, NMR, 3D microtomography) to understand the impact of the double porosity framework. Different polymers will be developed to investigate the role of the bulk material itself (e.g. hydrophilicity, plasticity, …).

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New Phenomena in Nanofluidics of Porous Media with Random Pore Structure

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The disordered nanoporous medium – non-wetting liquid system is actively researched for the development of impact/explosion energy-absorbing devices, accumulation of mechanical energy, thermal protection systems, nano-systems for the dosed drug delivery to the patient's body and in other perspective technologies. Dynamic phenomena which were observed in such systems are not described within the framework of traditional ideas based on the Laplace ratio, phenomenological angle of wetting and percolation nature of the intrusion – extrusion process. In the case of the non-wetting liquid, when the surface energy $\Delta\sigma > 0$, the liquid can fill a porous medium under the excess pressure. At subsequent reduction of the excess pressure (p) to zero non-wetting liquid should outflow from the medium under the surface forces. Recently, however, for some systems it has been found that at the initial filling $\theta>\theta c$, subsequent depressurization ($p = 0$) and at a temperature $T<Tc$, (θc, Tc – critical values) part of the liquid, or all liquid, can remain in pores of porous medium. From these critical dependencies on θc and Tc, it follows that the transition from the "non-wetting state" to the "wetting state" can be associated with the interaction of clusters of liquid in neighboring pores. It was experimentally approved that the relaxation of the "wetting state" (outflow of liquid) for investigated systems is abnormally slow and occurring at times of ~ 105 s and more. Dependence of the outflowed liquid volume on time (t) in the relaxation process obeys a power law $\theta \sim t^{(-a)}$ with exponent $a<0,1$. At $T>Tc$ and $\theta<\theta c$ nanoporous medium filling by non-wetting liquid may occur on a time scale $tin = (10^{-4}\div10^{-2})$ s and outflow of the liquid may occur on a time scale $tout = (10^{-2}\div10^{-1})$s. These dynamic phenomena are possible to describe as the properties of spatially inhomogeneous liquid state in a disordered nanoporous medium. As a consequence, the conventional interpretation of depending the pore volume filled by liquid on pressure is changed. These dependencies are used to determine the pore size distribution function. Change of energy (ΔE) of the inhomogeneous state with outflow (filling) the liquid from the pore is calculated in the quasiparticle approximation. The value (ΔE) is the sum of the energy changes in various local configurations of the emptying pore and her neighbors. Surroundings consist of z-n clusters of the liquid in filled neighbor pores and n empty pores (z - number of neighbors, $n\leq z$). Energy ΔEnz at $\Delta Enz>0$ is the energy barrier of the collapse of local configurations (z, n) at calculation $\theta(t)$ in the hydrodynamic approximation. From the analysis of the calculated energy spectrum (ΔEnz) and density of local configurations states it is should be relaxation mechanism of "wettability state". This mechanism corresponds to the scenario of self-organized criticality (SOC) of sequential collapse interacting local configurations. SOC scenario is implemented as a power law relaxation of "wettability state", observed for the studied systems. Supposed relaxation mechanism can also explain the difference between the filling time and the outflow time when the energy $\Delta E < 0$ and the "non-wetting state" is realized.

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Phase behavior of confined water in nanoporous organosilica hybrid materials with a periodically modulated surface polarity

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It is known that the properties of water in confined spaces with extents of a few nanometers will be altered and that for example the freezing/melting point can be shifted to temperatures below 220 K or completely suppressed. In addition to the geometrical confinement due to the pore size and topology the surface chemistry and therefore the pore wall properties play an important role because it determines the wettability/non-wettability of the nanoporous host structure. In a first step on the way to study the structural and thermodynamic behavior of water in ordered nanoporous structures the respective host materials will be presented. Several mesoporous silicas and organosilicas of the MCM-41-type with a narrow pore size distribution were synthesized using the liquid-crystal template approach. The obtained pore diameters were in the range between 2 and 5 nm. In contrast to the pristine silica the periodic mesoporous organosilicas (PMOs) contain organic bridging units (SiO1.5-R-SiO1.5) within the quasi-crystalline pore walls and therefore a periodically modulated surface polarity. The organic units R used were ethane, benzene, divinylaniline and biphenylene leading to an increasing length/thickness (5.8 Å, 7.6 Å and 11.8 Å) and hydrophobicity of the organic moiety within the pore wall. To study the thermodynamic properties of water in these confined spaces melting and freezing points of the inner pore water were measured by differential scanning calorimetric (DSC). The water loading of the porous samples was carried out in a climatic chamber with a glove door. All samples were loaded at 80 %RH for four days and sealed in the chamber. Besides the pore size the surface polarity is also influencing the melting point of water in the examined materials. The melting points of water in different PMOs are shifted by approximately 5-10 °C compared to the pristine silicas with the same pore diameter. This is probably due to the different adsorption and pore filling phenomena of water in these materials with localized more hydrophobic and therefore water repelling structural units. To obtain information about the localization of water in PMOs 1D and 2D solid state MAS NMR measurements were carried out. The pores of benzene-, biphenylene- and divinylaniline-bridged PMOs exhibit a quasi-crystalline long range order. Due to this there are two different regions in the pore walls which lead to a regular modulation of the surface polarity in the direction of the cylindrical pore channels. The change of the overall hydrophobicity as a function of the organic moiety was also shown by water vapor sorption experiments. Various solid state 2D HETCOR NMR (29Si-/13C-1H) experiments at different water loadings were applied to identify couplings between heteronuclear spins. The intensity of the cross peak depends on the distance of the two heteroatoms. A coupling can occur through bonds but also through space. When the HETCOR experiments were applied to benzene and biphenylene-bridged PMOs filled with water within the pores it was possible to determine whether the water protons are close to the 29Si nuclei and/or the 13C nuclei within a range of approx. 5 Å. The HETCOR NMR measurements reveal at certain degrees of water loading a coupling of the 29Si core and the water proton while in case of 13C-1H HETCOR NMR spectra no interaction of the respective nuclei was visible. This is a clear indication that the water is much closer localized to the inorganic regions of the pore wall than to the organic because of the different surface polarities and the non-wetting properties. This is contrast to the divinylaniline-bridge which can form H-bridges due to the primary amine group. Here one can detect water protons in close proximity to the organic moiety.

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Phase transitions in disordered porous solids

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Despite the notable progress attained in understanding the mechanisms of phase transitions in porous materials with ordered porosities, many aspects of these phenomena occurring in disordered porous solids still remain not fully explored. In this work we consider the simplest model of geometrically disordered materials, namely a linear chain of pores with different pore sizes connected to each other. For this pore space configuration we develop a statistical theory for phase transitions which takes account of the occurrences of both nucleation and phase growth processes. They are represented in the theory by their respective kernels which are available from the experiment or from microscopic theories developed for ordered pore systems. For the relatively long chains we obtain exact analytical solution in terms of the main transition pathways, such as adsorption and desorption isotherms obtained starting from completely empty and completely filled states, and of the scanning behavior, such as adsorption curves obtained starting from partially emptied and partially filled states, respectively. Notably, the framework developed is equally applicable for any transitions including condensation/evaporation, freezing/melting, and wetting/dewetting. We show that the predictions obtained using the theory developed for materials with different average pore sizes and pore size distributions reproduce the majority of the experimental observations reported in the literature for different porous materials, including also their scanning behavior. In particular, by sole variation of these parameters and of the chain length we naturally reproduce all hysteresis loops from H1 to H5 reported in the last IUPAC Technical report. Importantly, the theory provides deeper insight into the physical aspects behind the phase growth phenomena and may help in more accurate interpretation of the experimental data.

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Polypyrrole confined in porous silicon: From fundamentals to applications

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We investigate the properties of a functional filling of polypyrrol (PPy) in parallel, tubular pores of monolithic micro (pore diameter D < 2nm)-, meso- (2 < D < 20nm) and macroporous (D > 50 nm) silicon (PSi). On the one hand PPy offers the opportunity to modify the electrical conductivity of the PSi, while sensoric and actoric applications for the PPy/PSi hybrid system are possible as well. This leads to the investigation of the electrochemical polymerisation process of PPy into the PSi [1] with regards to the orientation of the molecules in the pores and the effect on the conductivity. Furthermore PPy is known to swell when exposed to a current in an electrolyte. The effect of the tubular pores on this behaviour and the influence on the mechanical properties, especially Young's modulus, of the macroscopic matrix can be studied with dynamical-mechanical analysis (DMA) and indenter measurements. This combined approach of a pore size dependant investigation of the molecular PPy structure within the pores as well as the mechanical, dynamical and functional properties aims at establishing the PPy/PSi as a model hybrid system.

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Prediction with Molecular Simulations of the Macroscopic Linear Strain Induced by the Water Content in Cement Nanopores

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Calcium-Silicate-Hydrate (or C-S-H) is the major binding phase in cement pastes and concretes and a porous hydrated material with a complex distribution of pores and molecular-scale spaces. This distribution controls the hysteresis of water sorption isotherms and associated bulk dimensional changes (shrinkage). In this work, we focused on the water sorption-induced strain in the smallest gel pores (<5 nm), since it corresponds to a scale where the overall mechanical properties of cement materials find their origin.

We performed grand canonical Monte Carlo simulations to compute water sorption isotherms in mesopores at room temperature (300K). Four sizes were considered (0.97, 1.46, 1.92, and 2.46 nm) to capture confinement effects on water sorption isotherms in C-S-H. Then, we computed the pore pressure for each of these molecular models.

Our results quantified the water content in the different pore sizes as a function of the relative humidity. Especially, we showed that for pores lower than ~1 nm, the water content remains constant on a wide range of relative humidity (from 10% to 100%). We also found that water sorption hysteresis appears in pores larger than 1.46 nm. Below that size, sorption mechanism is reversible. On a mechanical point of view, discontinuities at the capillary condensation and capillary evaporation correspond to a drop and a jump of the pore pressure of several tens to hundreds of MPa. Combining the aforementioned data on pore pressures with homogenization models, we predicted the macroscopic linear strain and we compared it with experiments.

These molecular simulations underscore the important role of confined water in modulating the structure and properties of calcium–silicate–hydrates upon exposure to various relative humidity.

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Properties of shale gas confined in nanoscale pores from atomistic view point by molecular dynamics simulation

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Shale gas (CH4) adsorption properties impose great influences on shale gas exploration and development, while the mechanisms from atomistic view point still remain unclear and deserve further investigation. In this work, adsorption properties of CH4 confined in nanoscale slit and cylindrical shale pores composed by kaolinite were firstly investigated through molecular dynamics simulations in NVT ensemble using Dreiding and OPLS force fields. The total and excess surface\bulk adsorption capacities were derived from CH4 density profiles along the direction perpendicular to the pore walls. The adsorption layer thickness, the percentage of adsorbed gas and the relationship between adsorption capacities with temperature, pressure, pore size and pore surface heterogeneities were analyzed. The boundary at which the gas is adsorbed versus free in the pore is defined. We found that the surface adsorption capacity increases exponentially with pore size less than about 10 nm and then slowdown to stabilization. The adsorption capacity decreases linearly with increasing temperature and can be fitted by Langmuir equation with pressure. The adsorption layer thickness is generally to be 0.9 nm and slowly effected by the pressure. The differences effected by pore surface heterogeneities on adsorption capacity is limited to a percentage of 15%. The percentage of adsorbed gas was dominated first by the pore size distribution and then the pressure. Then mass density of adsorbed CH4 was lower than that of liquid CH4 indicating that adsorbed methane is not liquefied. The simulation results were also compared with experiment and it proves that it is a good alternative method to estimate shale gas adsorption capacity by summation of accumulated molecules at pore surfaces by molecular dynamics simulation.

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Redistribution of water between nanometer-sized pores in hardened cement paste due to temperature change – a nuclear magnetic resonance study

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Thermal deformations of cement-based materials depend strongly upon their moisture state, i.e. on the degree of saturation of pores of different sizes. This is primarily due to the temperature dependence of sorption and it manifests in increasing relative humidity in the pores upon heating. This process is of paramount practical importance because drying cement-based materials experience higher thermal deformations (and therefore higher thermal cracking risk) compared to saturated conditions. However, the underlying physical mechanisms of the relative humidity increase upon heating are still under discussion [1].

In the present study, 1H nuclear magnetic resonance (NMR) relaxometry [2] has been applied to follow the redistribution of water between different populations of pores (namely pores in between the C-S-H sheets, gel pores within this cement hydration product and capillary pores, see Fig. 1) in hardened ce-ment paste caused by temperature changes. One of the major advantages of the method is that it uses water in pores as a probe itself, and therefore allows for in-situ, non-invasive and non-destructive test-ing. The results indicate that heating leads to immediate migration of water from the smallest interlayer pores (~1.5 nm) to the larger gel pores (~ 4 nm). The water exchange between these two classes of pores leads to an increase of the radius of the meniscus on the pore fluid-vapor interfaces (so-called Kelvin radius) and consequently to an increase of internal RH upon heating. This 1H NMR study is a first direct experimental confirmation of this mechanism.

Figure: Redistribution of water confined in different populations of pores (interlayer C-S-H spaces ~1.5 nm, gel pores ~4 nm, capillary pores ~tenths nm, see schematic representation on the right) due to temperature change as measured by NMR. The insert on the right is reproduced from [2] McDonald et al. Cem Concr Res 40 (2010): 1656-1663.

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Selective Adsorptivity and Capillary Condensation of Multicomponent Gases as a Consequence of Experimental Technique

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Understanding how the adsorption, desorption, and capillary condensation of multicomponent fluids occur is of fundamental importance to a wide range of industries, from pharmaceutical to petroleum. In spite of this, experimental data is scarce, and experimental inconsistencies make interpretation of that data difficult at best. Various methods have been reported for the study of capillary condensation in general. While evaluations of these methods as they pertain to experiments involving single-component fluids have been reported, there is no record of how different methods affect the capillary condensation of mixtures. To this end, we use a novel gravimetric apparatus to employ both static and flow-through methods to determine how the overall composition of the bulk fluid affects the composition and phase behavior of the confined fluid. In our study, we measure the adsorption isotherms of hydrocarbon gas mixtures in an 8-gram pack of MCM-41 with a pore size of 3.7 nm using both static and flow-through methods. In the static method, the overall composition of the fluid in our system remains constant, while the bulk phase is depleted of the more selectively adsorbed component(s). In the flow-through method, the overall composition of the fluid in the system is not constant, while the composition of the bulk fluid is constant. The methods inherently result in different confinement-induced shifts of the phase diagram. To pursue our objective of gaining a comprehensive understanding of how capillary condensation and confinement-induced phase behavior affect the storage and production mechanisms of ultra-tight gas reservoirs in the petroleum industry, we propose the flow-through method as the most appropriate method for further studies into reservoir-conditions experiments.

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Simple fluids confined in nano-slits: from local transport properties to shear-swelling couplings

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1) Introduction Dense simple fluids confined in nanoslit pore are generally strongly inhomogeneous due to layering of the molecules of the fluid because of adsorption and molecular packing [1]. In such nanoporous system the confined fluid exhibits local and effective transport properties that may strongly differs from those of the bulk [1-3]. Furthermore, this extreme confinement can induce as well strong solvation forces on the solid matrix that may lead to swelling/shrinkage as well known in clays for instance.

2) Methodology To improve the microscopic understanding of the phenomena described above, we have performed extensive molecular dynamics simulations on simple fluids confined between flat solid surfaces. In all cases the solid phase has been modeled using a rigid CFC crystal composed of Lennard-Jones atoms. Concerning the fluid, different molecular models were employed, from hard sphere to Lennard-Jones, so as to build new weight functions for a non-local model for transport properties based on a local average density model. Furthermore, to ensure the reliability of the model so obtained, various thermodynamic conditions have been explored. Various non equilibrium molecular dynamics scheme have been developed [2-4], see Fig. 1, in order to study the impact of extreme confinement on the confined fluid properties.

3) Results and Discussion We will show how the local variations of the transport properties of the confined fluid (diffusion [1], viscosity [2]), induced by density inhomogeneities, can noticeably affect the effective transport properties of the fluid quantified at the pore scale. Furthermore, it will be shown that these local transport properties can be essentially described by a simple local average density model combined with simple weight functions [3], see Fig. 2. In addition, we will discuss the couplings that occur between shear and swelling at the pore scale because of the strong fluid structure [4]. It will be shown that shear can induce swelling and vice versa because of the confined fluid phase structure, see Fig. 3. This implies that the response to a variation of the external load is a combination of volumetric and shear deformations, because of the fluid. These phenomena, which are usually neglected in poromechanics modeling, may be non-negligible in highly structured microporous systems such as cementitious or clay-based materials [5].

Figure 1: Scheme of the molecular dynamics simulation cell used to study couplings between shear and swelling (green: fluid particles, red: solid particles) [4].

Figure 2: Variation of the local shear viscosities perpendicularly to the solid wall [3].

Figure 3: Variation of the distance between the solid surfaces with time during boundary shear [4].

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Sol-gel films and their properties related to nanoporosity.

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Complex hierarchical nano structures can be achieved when combining chemical advanced bottom-up strategies, such as self-assembly and sol-gel chemistry, together with liquid solution processing. Amongst them, dip-coating is an extremely versatile tool to prepare thin nanostructured and mesoporous metal oxide films from liquid solutions and has been used for many decades without taking advantage of its whole potentiality. [1,2,3] This communication reports on the recent progresses performed in nanostructured porous sol-gel metal oxide coatings, and on the investigation of their porosity using elliposmetry porosimetry. The critical effect of pore characteristics (pore dimension, pore volume and pore constriction) on capillary infiltration of liquids in mesoporous films will be discussed. [4] Finally, the evolution of the internal stresses related to water adsorption and capillary condensation in microporous and mesoporous films will be presented together with their associated humidity-sensitive actuating properties. [5]

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STRUCTURAL TRANSFORMATIONS OF METHANE ADSORBED IN NANO-PORES

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Structural transformations of nano-systems show properties different from their 3D bulk analogs. The mechanism of transformation is different due to the nano-object size or nanometric confinement. This field has not yet been fully explored and requires more fundamental studies which may lead to future application, e.g., in nano-porous systems characterization. Properties of methane adsorbed in confined geometries are interesting from both fundamental and practical points of view. At ambient temperatures super-critical adsorption is studied for possible methane storage applications. At the same time, the analysis of methane's low temperature adsorption properties is essential for understanding the mechanism of adsorption as a function of temperature, pore size, pore topology and heterogeneity. The temperature dependence of structures of adsorbed phases allows one to understand evolution of confined phases in nano-space. In this work we compare the mechanism of adsorption and structural transformations of methane confined in (i) homogeneous carbon slit pores of widths between 1nm and 4nm and (ii) heterogeneous MOF pores. We discuss the mechanism of layering transition, melting and capillary condensation in sub-critical conditions, for temperatures between 80 K and 180 K. The mechanism of layer formation is strongly temperature dependent. At the same time, a commensurability between the methane and the pore sizes is important factor. In slit pores it evolves from a sharp layers formation at 80 K to continuous adsorption at higher temperatures. The capillary condensation is observed clearly in slit pores bigger than 2 nm. The melting transition of methane in slit pores shows complicated mechanism where the interior of the pore melts at lower temperature than the layers adsorbed closer the pore wall. We compare this behavior with the mechanism of adsorption in MOF porous structures where the adsorbing walls are strongly heterogeneous both structurally and energetically. The comparison between the slit pores and the MOFs will allow us to discuss an influence of the heterogeneous wall topology and inter-molecular interactions on the thermodynamic properties of nano-confined structures.

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Structure, Dynamics and Phase Behavior of a Discotic Liquid Crystal Confined in Nanoporous Anodic Aluminum Oxide Membranes

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The interest in porous anodic aluminum oxide (AAO) has been rapidly growing due to its numerous applications in separation, catalysis, energy generation and storage, electronics, and sensors [1]. From the scientific point of view, AAO is a topical interest in soft matter fields. Spatial confinement of soft matter in nanoporous media influences its structure, thermodynamics, and mobility [2]. Embedding polymers and liquid crystals into nanopores of AAO results in a 2D nanoconfinement of these materials. This confinement affects their properties, compared to the bulk, such as phase transition temperatures and enthalpies, molecular mobility, and architecture of the crystallization [3,4,5]. On the other hand, discotic liquid crystals (DLCs) are a promising class of soft matter for electronic applications. This is due to their ability to organize and stack themselves into columns in a hexagonal columnar mesophase, a mesophase in between the plastic crystalline and isotropic phase, driven by the overlap of the π orbitals of their aromatic core. This leads to a high charge-carrier mobility along the column axis. Further, these columns could then be considered as “molecular nanowires” [6]. Here in this study, 2,3,6,7,10,11 hexakis[hexyloxy] triphenylene (HAT6), a triphenylene based DLC, was confined into nanoporous AAO membranes. The structure, dynamics and the phase behavior of the confined HAT6 were investigated by broadband dielectric spectroscopy (BDS) and differential scanning calorimetry (DSC). HAT6 was embedded into nanoporous AAO membranes by melt infiltration in the isotropic phase under argon atmosphere. The membranes have parallel aligned cylindrical nanopores, with pore diameter of 10, 20, 25, 40, 80, 120 and 180 nm. The filling degree for each sample was checked by thermogravimetric analysis (TGA) in order to ensure complete filling. Bulk HAT6 forms a hexagonal columnar phase; in between the isotropic phase above 371 K and the plastic crystalline phase below 340 K. Unlike the bulk, the confined HAT6 split the plastic crystalline-to-hexagonal columnar phase transition in two, which might be interpret as two different phase structures; close to the wall and at the pore center. Moreover, the isotropic-to-columnar transition of the confined HAT6 shifted, with decreasing pore diameter, to lower temperatures. Furthermore, pore surfaces of a series of membranes were chemically modified, resulting in a more hydrophobic pore surface than the unmodified ones. HAT6 was embedded into the modified membranes by the same aforementioned preparation. The influence of the changed host-guest-interaction, on the structure, dynamics, and the phase behavior of HAT6 confined in the modified membranes, was also investigated by BDS and DSC.

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Surface Effects on Triple Point Behavior of Ar and N2 in Mesopores

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The properties of fluids under confinement have gained significant interest due to their application in a wide field of processes, ranging from gas storage and separations to sensing devices. Bulk vapour, liquid and solid phases are well defined by the Gibbs phase rule and co-exist in equilibrium at the bulk triple point (T3). On the other hand, when matter is confined within a material with pore sizes of a few nanometers, the system's behavior is different than the bulk. Phase boundaries are no longer clearly identified and phase transitions are shifted because of stronger, attractive adsorbate-adsorbent interactions, compared to intermolecular forces. Although pore condensation (i.e gas-liquid transitions) has been studied in detail, freezing of confined sorbed fluids as well as gas-solid equilibria in porous materials are still in need of further investigation. In order to investigate the effect of confinement on the phase behavior of Ar and N2 below T3 a series of sorption experiments were performed at different temperatures (above and below T3) on a mesoporous as-etched silicon membrane and its surface oxidized (H2O2 treated) analogue. The samples have similar pore sizes, however the sorption isotherms revealed a fundamentally different pattern below T3, highlighting the critical role of pore surface chemistry on the phase properties. In brief, both samples revealed similar gas-liquid transitions above and slightly below T3. However, upon further cooling, solidification was only possible in the pure silicon sample indicating that the solid phase is unstable when the surface is oxidized (-OH rich).

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The Effect of Nano-Confinement on the Densities of Multicomponent Fluids for Applications in Hydrocarbon Gas Recovery from Tight Reservoirs

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Despite their growing significance as important energy resources throughout the world, shale gas reservoirs are still not well understood. In particular, the thermodynamic behavior of gas at reservoir conditions cannot be accurately modeled, underscoring the lack of knowledge as to how gas is stored in and produced from shale reservoirs. Due to the nanoscale confinement of the gas in organic-rich pores, we hypothesize that the gas is stored at a higher density than what is normally encountered in the bulk for the same temperature and pressure conditions. We present the results of a preliminary investigation into this hypothesis by monitoring the densities of multicomponent hydrocarbon gases in nanoporous media over a variety of temperatures and pressures. We then compare those densities to the bulk values of the same fluids at the same temperatures and pressures. To determine the densities of the confined fluids, isotherms for the fluids are used in conjunction with precise geometrical knowledge of the adsorbents. Isotherms are measured in 8-gram packs of adsorbents using a novel gravimetric apparatus to determine the mass of fluid, while the geometries of the same packs are used to calculate the volume of confined fluid. For precise volume calculations, information about the nanoporosity, macroporosity, and total porosity of a given adsorbent pack is utilized. Values for nanoporosity are derived experimentally from nitrogen adsorption, X-ray diffraction, and transmission electron microscopy. The macroporosity of each adsorbent pack is deduced from data gathered from high-pressure adsorption experiments. Bulk porosity is calculated from the CT numbers of tomographs of each adsorbent pack taken using a medical CT scanner.

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The influence of micropores and organic residues on the adsorption-induced deformation of hierarchical structured porous solids

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Silica monoliths with hierarchical porosity were used as a model system to investigate adsorption-induced deformation as a function of humidity at the macro- as well as the mesopore scale [1]. Therefore, we combined in-situ dilatometry with in-situ small angle neutron scattering (SANS) to simultaneously examine the strain of the sample on both length scales. For the measurements at the SANS-1 instrument (MLZ Garching, Germany), a sample holder was designed accommodating a thin slice of the silica monolith to be analysed. The water used for the adsorption was partially deuterated to make the adsorbate invisible to the neutrons (zero scattering length density). This allows for the determination of the strain within the mesopore lattice without the influence of strong contrast effects usually experienced with X-rays when investigating systems with partially filled pores [1,2]. Prior to the in-situ experiments, water adsorption isotherms were recorded to determine the relative pressure regimes of particular interest, i.e. the points of capillary condensation and evaporation. Three different samples were investigated: the first sample was used “as prepared”, the second sample was calcined to remove residual organics of the synthesis process (thus creating micropores) and the third sample was additionally sintered at 750°C to significantly reduce the micropore volume. Small-angle X-ray scattering (SAXS) and N2 adsorption measurements on the evacuated samples reveal that the structural changes due to the post-treatments were minor at the levels of macro- and mesopores but severely influenced the microporosity. Both in-situ techniques show that the maximum strain during water adsorption differs by almost an order of magnitude, being largest for the “as prepared” sample and smallest for the sintered sample. This indicates that the adsorption-induced deformation of the samples investigated is dominated by effects taking place within the mesopore walls, i.e., in the micropores of the calcined sample and the organic residues of the “as prepared” sample.

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The model of disordered porous medium taking into account the many-particle correlations of pores

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The scientific and technological problems of disordered porous media, one of the most actively researched areas in physics today. Questions about heterogeneous nature of local areas, the correlation in the arrangement of the various far, their causes and metastability, their relationship with nature and mechanism of anomalously slow relaxation in disordered glassy, including disordered nanoporous environment remain unclear. The solution of these problems can lead to serious technological breakthrough, due to the fact that the systems of the large nonlinear response to external changes (in particular on the temperature increase) can be used in drug delivery systems, sensor with high temperature sensitivity, passive protection systems such as in fire protection systems, in systems with controllable permeability for liquids or gases. Information about the correlations will take a fresh look at the heterogeneous catalysis and mercury porosimetry.

The paper proposed a model of the medium taking into account the many-particle correlations of pores. The mudium consists of randomly arranged intersecting spheres of different sizes. The space of pores is voids within spheres. In this model the number of nearest neighbors analytically calculated, that in the future will restore the function of the pore size distribution based on their correlations.

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The relaxation of metastable state method for recovery of distribution of captured non-wetting liquid dispersed in nanoporous medium

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More than twenty years a lot of scientists study of non-wetting liquid entrapment phenomenon [1, 2]. This phenomenon is observed not only for disordered porous media [2], but also for porous media with an ordered structure, such as MCM and SBA type materials [2, 3]. In recent years have been found effects during intrusion - extrusion non-wetting liquid process such as the existence of metastable states [4] and their power law relaxation [5]. The methods have been described in this works will provide information about quantity of captured non-wetting liquid in porous media and changes of quantity of liquid captured in porous medium in time. Results of investigation intrusion - extrusion non-wetting liquid process for several nanoporous media by the metastable state relaxation method were presented. The experimental results were used for determination of the pore size distribution for pores from which non-wetting liquid does not outflow after reducing the excess pressure to zero.

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Transport of Hydrocarbons Mixtures in Shales Subnanoporous Matrix

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Despite the recent major focus on shale-gas, no model has been provided to understand the transport of hydrocarbon mixtures in shales subnanoporous matrix (kerogen). Since continuum descriptions such as Darcy's law cannot be used to describe transport of linear alkanes through subnanoporous carbon membranes (pore size below 2 nm), we use molecular dynamics and statistical mechanics to rationalize the behaviour of both equilibrium and non-equilibrium transport coefficients of hydrocarbon mixtures. As kerogen replicas we use the realistic numerical model of kerogen's microporosity developed by Bousige et al. [1]. Under applied pressure gradient, the velocity of each component of the mixtures at steady-state is still proportional to the pressure gradient. The coefficients of proportionality, called permeances, depend on the density and on the solid-fluid interactions. We use the Fluctuation Dissipation Theorem in order to derive a Green-Kubo relation between the permeances and the Onsager coefficients that can be evaluated at equilibrium. Due to strong adsorption effects, it appears that the hydrocarbon transport behaviour is mostly influenced by the interactions with the microporous matrix. As a consequence, the permeances of the different components of the mixtures scale in a simple way with the alkane length, independently of the nature of the mixture (number of components, composition). Moreover, this scaling is the same as for the pure component case described previously [2] with a free volume theory. The effects of the solid-fluid interactions and of the crowding on the transport are decoupled and captured respectively by a friction and an overlap coefficient that can predicted from the pure component case [3]. To get further insights on hydrocarbon transport in kerogen, we investigate how these coefficients can be linked to the topology of the host matrix. We aim at proposing simple relations between the transport coefficients of the free volume theory and the porosity of the kerogen's microstructures.

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Water Transport Through Anodic Aluminum Oxide Nano-Porous Membranes

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Darcy flow is the prominent mechanism of fluid transport, which is based on the continuum representation of the porous media. However, liquid transport in nano-scale porous formations, such as those observed in shale reservoirs, can exhibit substantially different physics than what is observed in larger-scale systems. In nano-scale confinements, atomic interactions between liquid and wall molecules may lead to velocity slip, no-slip or liquid adsorption on the walls [1]. In addition, molecular simulations have shown strong liquid density layerings near the walls, where transport coefficients such as viscosity may not be defined based on the local thermodynamic state [1]. At smaller scales, even the constitutive laws that determine the stress tensor may breakdown [1-3], and therefore, it is necessary to investigate transport in nano-porous media theoretically and experimentally. Motivated by the development of transport models in nano-porous media, we present an experimental study that focusses on pressure driven flow of deionized (DI) water through 10 nm – 40 nm pore diameter Anodic Aluminum Oxide (AAO) membranes. We particularly focus on AAO membranes due their well-defined pore-geometry. The AAO membranes have elliptical or circular pores that extend straight like a pipe across the 50 µm thick membrane (ie., tortuosity of unity). Using SEM pictures taken before and after the experiments, we carefully characterized the AAO membrane geometry, determined pore diameter and its statistical distribution. We also determined the pore-density and porosity of the membranes. Comparisons of SEM pictures taken before and after the experiments are used to explain any possible pore size reductions due to multi-layer adsorption or chemical interactions between DI water and AAO membrane surfaces. Simple geometry enables direct comparisons of experimentally obtained volumetric flowrates and predictions from the Poiseuille flow formula with or without slip-correction. We investigated pressure driven DI water flow thorough 10 nm, 20 nm and 40 nm diameter AAO membranes. Experiments were conducted by measuring the mass flowrate under systematically increased and then decreased pressure gradients. Flowrate is measured by accumulation of water exiting the system as a function of time using a high precision scale. Linear relationship between the mass flowrate and pressure gradient are validated for each experimental set. Three different sets of experiments are conducted for each membrane within three consecutive days to assess repeatability of the data and observe possible time-dependent variations on the AAO pore surfaces. Although our experiments are still continuing, most results to this date have shown 2 nm reduction in the pore diameter, which can be explained as velocity stick or multi-layer adsorption. In fact, water-AAO surface binding energy is very strong [3-5]. The equilibrium water contact angle of AAO surface is examined by us and others [4-5], and found to be less than 30o, indicating almost super hydrophilic behavior. We plan to present our experimental results, and support our observations with MD simulations and the phenomenological continuum model in [6].

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Different tectonic coals adsorption and desorption laws experiment research and enlightenment

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The isothermal adsorption and desorption laws were investigated using the same volume lump coal samples including undisturbed coal, cataclastic coal; flaky coal and mylonitic coal all taken from Hancheng mining area with self-developed lump coal isothermal adsorption and desorption test device. In this experiment process, using lump coal to gas in the coal body flow contains a complete "seepage, diffusion, adsorption or desorption " 3 links, more in line with the actual flow condition of the gas in the underground coal seams. The results show that: the undisturbed coal gas adsorption and desorption characteristics is the worst. Although the mylonitic coal on gas adsorption and desorption efficiency is highest, and can finish in a very short time, this is primarily because the gas is attached only in the pores within a certain range of the "outer surface" of the lump mylonitic coal. Cataclastic coal and flaky coal gas adsorption and desorption process presents a fast to slow variation, especially the adsorption and desorption volume are the highest. On the basis of the above experimental conclusions and from the point of coal seam gas development perspective can get the following enlightenment: the compact undisturbed coal is the negative areas of exploitation of coal seam gas. Mylonitic coal on gas has obvious "sealing" effect, is the unfavorable reservoir for the exploitation of coal seam gas. Cataclastic coal and flaky coal internal fissures developed very well to have a persistent gas production and total yield advantage, is the most favorable reservoir for the exploitation of coal seam gas.

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Effective flow properties assessment of a propped fracture under in-situ conditions – numerical modeling

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Hydraulic fracturing treatment is widely used to maintain the production of oil or gas from low permeability formations. The main goal of hydraulic fracturing is to create a network of highly conductive pathways in rock and increase the surface of the reservoir that is connected directly to the wellbore. Injected proppant grains keep fracture open against the normal stress after fracking is finished. In our considerations, we assume that fracture is filled with a partial monolayer of propping agent, which is desirable in shale reservoirs (Brannon et al. 2004).

Flow patterns in propped fractures govern transport processes during production stage and determine the effective exchange surface between the fracture and matrix. Our aim is: firstly, to understand microscopic scale flow behavior for a small fracture region with one or tens of proppant grains using 3D numerical simulations; secondly, reduce the flow equation over the fracture aperture and compare it against 3D numerical model; and finally, use the flow model to obtain effective flow and transport properties of the medium and further upscale the results to the reservoir scale.

A fracture made of two parallel plane walls is considered. The void space between the fracture walls is filled with a partial monolayer of proppant grains. As the fracture experiences closing pressure, proppant grains can deform and/or embed into the impermeable rock matrix. To take this effect into account and simplify the model, proppant grains are approximated with cylinders placed between the two fracture walls (Figure 1a – shows the geometry of a propped fracture). Macroscopic pressure gradient is applied to drive a creeping flow of a single-phase, incompressible fluid along the fracture. Stationary velocity field is obtained by solving the Stokes equations discretized using the finite element method on a body-fitting tetrahedral mesh (Figure 1b – shows the geometry and calculated velocity magnitudes). More details about the solution method can be found in Dabrowski et al. 2008.

As numerical calculations in three dimensions are computationally demanding, we reduce the Stokes equations to two dimensions and discretize them using triangular meshes. To take into account a finite fracture aperture, we use Stokes-Brinkman equation (Brinkman 1947). The Stokes-Brinkaman model allows us to use no slip boundary conditions on the grain surfaces, which is a major improvement over the Reynolds lubrication approximation.

Systematic simulations using the 2D Stokes-Brinkman model were performed. Periodic boundary conditions were used to minimize boundary effects. The effective medium properties are studied as a function of proppant fractions and fracture aperture to proppant grain diameter ratios. Figure 2 shows the velocity field for a fracture propped with 1000 grains for two different values of the fracture aperture to proppant grain diameter ratio (b/d). For low ratios, the flow patterns are quite dispersed, for high values flow paths are strongly preferential, which may have a significant influence on transport properties.

More systematic results are presented in Figure 3, where effective transmissivity in direction of imposed pressure gradient is plotted versus proppant packing fractions for various fracture aperture to proppant diameter ratios (b/d).

Figure 1 Geometry of a propped fracture (a) and velocity field computed in fracture with 128 proppant grains (b - left) together with zoom of selected region of the sample (b - right).

Figure 2 Velocity field in selected region of sample with 1000 proppant grains for b/d = 0.1 (a) and b/d = 0.5 (b).

Figure 3 Effective transmissivity of a fracture with 10 000 grains as a function of proppant fraction for b/d = 0.05 (circles), 0.25 (squares) and 1 (triangles), by black solid lines are plotted approximated solutions obtained by Differential Effective Medium theory scheme.

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Grain-scale modelling of swelling granular materials: the effect of particle shape on porosity, permeability and retention properties

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Swelling of porous materials is a common and important phenomenon in earth materials and industrial products; for example, in paper, hygienic products, and swelling clays. Hydraulic parameters of hygienic products, such as porosity, permeability, and retention curves depend on the degree of swelling of the Super Absorbent Polymer (SAP) particles. SAPs can swell up to 30 times their initial mass, most of which occurs in less than 5 minutes. Therefore, change in hydraulic parameters during swelling cannot easily be identified by experiments unless a quasi-static approach is used. To overcome this problem, we have performed grain-scale simulations of compaction of SAP particles to reconstruct the pore geometry for varying degrees of swelling and various degrees of compaction, using the Discrete Element Method (DEM). To obtain large porosity values (>0.45) of typical SAP packings, the shape of individual particles is included. This was achieved by approximating the shape of a non-spherical particle by an assembly of spheres, called a clump of spheres. The real shape was obtained using micro-CT scans of individual SAP particles. Then, the individual particle shapes were extracted and exported into surface plots. Using the surface plots, around 14 spheres were randomly fitted into each particle by employing a fitting algorithm. Finally, we obtained a library of 20 particles which are represented by clumps of spheres. In DEM, particles were then randomly generated using the particle shape library and based on the particle size distribution of SAP. The particle packing was then compacted under a constant confining stress. The resulting pore geometry was used to obtain the retention properties using Pore Morphology Method, and the permeability using direct simulations. The major advantage of this method is that we can perform dynamic simulations in DEM, where by particles can swell over time, while measuring various hydraulic parameters.

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Improving methane drainage in low-permeability coal seam using the water jet technique

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Approximately 69% of coal seams in China have low permeability. The desired drainage effect is frequently difficult to achieve with the traditional methane drainage method. Our experiment shows that stress is a key factor that affects the permeability of coal seams. In addition, vertical stress is greater than horizontal stress. This study proposes using horizontal continuous water jet cutting to reduce vertical stress seams and create artificial fractures that can significantly increase the permeability of coal seams and improve methane drainage efficiency. According to the results of the project application, the accumulated gas exploitation volume of the slotted hole in the original coal seam is 2.2 times that of traditional drilling. Meanwhile, the speed of the former is 2.5 times that of the latter. When affected by mining action, the gas emission speed of the slotted hole is 15 times that of traditional drilling.

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NMR imaging of bound and free water transport during wood imbibition and deformation

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Introduction.

During water imbibition in wood, moisture penetrates not only in liquid form (free water) into the pores of wood, but a fraction of water molecules is also absorbed within the cell walls (bound water) inducing the swelling of the wood material. Although wood-water interaction has been studied for decades, the dynamics of water transport during imbibition and its interplay with bound water and deformation are still poorly known, in particular due to a lack of direct internal observations. Moreover, some curious facts have been observed and studied, for example, the permeability depending on the sample length [1] is in contradiction with Darcy's law which a priori describes liquid transport through a homogenous porous medium. Our original experimental approach, allowing to follow at the same time deformations and bound and free water, makes it possible to clarify some aspects of this problem.

Materials and methods.

Wood samples are collected from a poplar trunk with 10 cm in longitudinal direction (parallel to the imbibition direction). The bottom of samples is immersed in water with about 1cm in depth and the imbibition process is followed up to 3 days. Tangential and radial deformations are also measured along the imbibition direction at different times. The distribution of water content along the sample axis is measured by a 0.5T 1H MRI spectrometer with a one dimensional multi-echo sequence (CPMG sequence) which has been especially developed to allow distinguishing bound and free water in wood taking into account the NMR relaxation times of each type of water. This technique allows, as far as we know, for the first time, to observe separately the dynamics of both water phases. We also carried out standard 2D density imaging to observe the transversal distribution of (free) water.

Results.

As previously observed [2] 2D images show that the water penetrates in some preferable zones but at different rates in different growth-rings, which reflects the heterogeneity of the system. Our 1D MRI profiles of the distribution of free water (continuous lines in Fig.1, every 6 hours) per unit section area along the sample axis shows that this water advances as a front keeping the same shape. This process seems to correspond to a Washburn imbibition (here the saturation front is not straight due to system heterogeneity). Bound water (short dash lines in Fig.1) spreads in a very different way throughout the sample: it advances more rapidly than free water and reaches the sample top much before the bound

water saturation. This propagation has some similarity with that obtained from diffusion from a source maintained at a given concentration. Finally, the deformation profiles (square symbols in Fig.2), represented in terms of water volume per unit area, are compared to bound water profiles (continuous lines in Fig.2). Remarkably the dynamics of bound water is directly correlated to that of the deformation (see Fig.2): both profiles have a similar shape and evolve approximately with the same timing. This clearly confirms that the macroscopic deformations of wood are intimately linked to bound water diffusion.

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Shocking Hydrogels – Time evolution of a spherical hydrogel in respons to an osmotic shock

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A fully swollen polyacrylamide hydrogel is suddenly brought into contact with a dextran solution. Due to the dextran osmotic pressure water flows out of the gel. The dextran subsequently diffuses into the gel, decreasing the osmotic pressure. Using a large deformation model we calculate the change in volume of the hydrogel as a function of time and establish the permeability of the gel and the dextran diffusion constant inside the gel network. In the limit of small osmotic shocks the gel deformation may be calculated analytically.

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Stress and Saturation Dependent Hydro-Mechanical Properties in Organic-Rich Eagle Ford Reservoir Shale and Seal Shale Pierre

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Shales have hydro-mechanical properties attributed to their complex nano-scale pore characteristics along with various clay minerals and organic-rich composition. In nano-porous media, fluid transportation complexity is increased as a result of exclusion of solute molecules dissolved in solution due to organic-rich components, rock-fluid interactions, and capillary condensation. Development of reliable geomechanical models in shale formations is of great interest for reservoir characterization, wellpath optimization, efficient drilling, cementing, well completions, and production from conventional and unconventional reservoirs as more than seventy percent of the formations drilled are shale formations in addition to the recent advancements made in gas and oil production from tight oil and gas shale reservoirs. The mechanical properties of low permeable structures of shales need to be described by being coupled with pore fluid behavior. Pore-scale structure of shale is anisotropic due to lamination of mineral grains deposited in gravity, preferential distribution of microcracks along the bedding planes, and stress-induced anisotropy. Stress alterations in the reservoir caused by the drilling and hydraulic fracturing operations have a significant impact on the mechanical properties. In addition, fluids used for hydraulic fracturing with various chemical additives can largely alter the hydro-mechanical properties of shales sensitive to disturbance in electrochemicalforces. Therefore, coupled measurements and modeling capturing these effects simultaneously will reflect more realistic formation responses. Experimental data revealing the coupled response of hydro-mechanical properties are very limited as measurements take time to stabilize the stress state in shale for transmission of pore pressure and dissipation of excess pore pressure. In this study, we report organic-rich Eagle Ford shale laboratory data measured in a triaxial pressure cell assembly enclosed in precisely-controlled temperature condition to obtain stress-dependent permeability and mechanical properties. Pierre seal shale measurements were also conducted in the same stress state and temperature conditions in order to determine the difference and similarities between the reservoir and seal shales. The Pierre shale has significantly high smectite content of approximately 60% while the reservoir shale tested is calcite rich with quartz and about 10% kaolinite clay content. The comparison of both reservoir and seal shales illustrates existence of a higher stress sensitivity of permeability and wave velocities in the reservoir shale. The effect of fluid injection on compressional and shear wave velocities was investigated. A preserved core sample of Eagle Ford shale was loaded up to 45 MPa at 13.8 MPa of nitrogen pore pressure and subsequently subjected to injection to 1,000 ppm NaCl solution. Another twin core sample was used to expose the sample to 60,000 ppm KCl solution at 24 MPa of mean net stress. It is observed that the final velocity-stress dependence was not sensitive to the stress path and fluid injection history as illustrated in Figures 1 and 2. The pore fluid effect was evident in the compressional wave velocities measured while shear velocity showed no dependence on the fluid injection. Further comparison on the relationship between the injection fluid, wave velocities and permeability in the reservoir shale and seal shales will be discussed in the full paper.

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Study on Coal-bed Methane Absorption/Desorption of multi-physical coupling effects

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For the industry project and technology of coal-bed methane exploitation, super-heated water or vapor was adopted to be injected into coal seam afterwards so many fractures were shaped. The paper was stated theoretical study, meso-permeation of two phase fluid mechanics experiments, macro-large scale coal samples in laboratory on different temperature and water pressure of methane adsorption or desorption experiments, and micro-small scale coal specimen corresponding with laboratory ones in numerical studies. Finally, the adsorption or desorption law of coal-bed methane influenced by multi-physical coupling effects such as water and temperature was studied. And the results are presented in following items. The viewings of coal absorbed methane and high pressure water injection experiments under micro CT were observed. It is presented for the coal specimen of 2 mm×2.5 mm×10 mm and showed that once coal specimen adsorbed methane, the porosity was decreased about 3% at the same zone and the tendency was not obvious followed by gas pressure increased. Once after water injection, the porosity was also decreased about 4% at the same zone. If external water unloaded, the porosity was still decreased. The adsorption - water injection - desorption testing machine was manufactured by own for room temperature (20oC) desorption characteristics experiments of high pressure water injection after adsorption methane using direct cylinder raw coal sample, the results presented that: the natural desorption law of experimental coal sample is the same as actual coal mine. Desorption percentages (PD) in different water injection conditions are obeyed one time effect formula, the value is determined by critical value of desorption time effect t0, the law is more water pressure, larger the value. Desorption characteristics of methane bearing coal sample are mostly influenced by water, PD are only 50-70% times to natural at equality water pressure with gas pressure. Followed by water injection pressure increased, final PD is relative with water pressure. Combining porous distribution law of coal samples, the critical pore size-scale of water into coal sample was calculated in different water pressure. The smaller is critical value, the lower is PD. And PD of coal sample is related with equilibrium adsorption methane pressure and porous distribution law of coal. For the temperature raised (30-110oC) desorption characteristic experiments of coal sample in high pressure water injection after adsorbed methane, the results presented that: desorption capacity of methane bearing coal sample after water injection is improved as a function of temperature rose. Desorption will reach saltation once up to or exceed boiling point of water. And the PD in 90oC after water injection is still larger than natural PD. There is a function relationship between PD and temperature; they are related with liquid activity and surface adsorption potential. For the methane adsorption experiments of water bearing coal sample and the results presented that: the methane adsorption capacity will decreased after block coal sample adsorbed water. It is existed functional relationship between adsorption capacity and moisture rate. For the high temperature (30-270oC) desorption characteristic experiments of methane bearing coal sample, the results presented that: the decreasing velocity of adsorption in fixed volume experiments is decreased with temperature rose; increasing velocity of equilibrium adsorption gas pressure is increased with temperature rose. The decreasing velocity of adsorption in fixed pressure experiments is increased with temperature rose. In experimental temperature (30-270oC) and gas pressure (≤7MPa), the adsorption is still the first one of coal absorb methane and would be reach maximum value once up to definite gas pressure at the constant temperature. It is defined the single molecular adsorption model.

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Taking Time Out of the Picture: Capillarity and Permeability Behaviors in Swelling Mixtures of Fluff and Superabsorbent.

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The flow, distribution and retention of fluid in an absorbent pad of cellulose fluff fibers mixed with superabsorbent hydrogel particles depends on porosity, capillarity and permeability in the pad. While detailed, time-dependent models of swelling porous media can be used to follow flow as fluid is added to the pad, patterns in structure properties like porosity can also be deduced by tracking swelling levels of fibers and particles over a range of time-independent swelling paths. For example, the conventional trade-off of capillary-pressure increase and structure-permeability decrease due to swelling is readily apparent when plotted on swelling paths. The volume change of gel spheres (up to 20X) can be contrasted to the surface-area change of cylindrical fibers for alternative models of permeability or capillarity. Comparison of different paths allows the influence of fiber and particulate swelling to be followed even down at the level of the pore distribution for the interstitial space. To encourage further activity in such mixtures of swelling components, several open challenges in modifying fluid distribution are laid out against the fundamental patterns of behavior shown in swelling-path plots.

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The coffee press: rapid deformation of a highly deformable porous medium

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The phenomenon of coupled flow and deformation in porous media arises in a huge range of settings. In particular, the role of the 'dewatering' of deformable media or dense suspensions is extremely important in the mining, waste treatment, and pulp and paper industries. This presentation will explore one-dimensional compaction of a highly deformable medium by a porous piston, focussing in particular on the spatial variations in flow and deformation that arise under very rapid compaction. The results of a mathematical model will be explored, and the qualitative behaviour of the suspension for different constitutive models will be discussed. Model results will be compared with detailed experimental measurements from compression tests on various fibrous media, with a particular focus on cellulose fibre suspensions. It is found that the model gives an excellent agreement with measurements for idealised nylon fibre suspensions, but shows qualitative differences when compared to cellulose. This discrepancy can be removed by the addition of a viscous-like dissipation in the fibre rheology, which is justified based on the microstructure of cellulose fibres.

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A constitutive model of unsaturated soils with considering the effect of intergranular physicochemical forces

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A clayey soil is an electrically charged porous medium, and its behavior is sensitive to the composition and concentration of the saturating fluid. Pronounced physicochemical interaction can occur between the solid particle and the pore fluid, so that the clayey soil shows strong chemo-mechanical coupling effect and complex mechanical behavior. When the saturation varies from 100% to a low extreme, the composition and concentration of the pore fluid are variable, resulting in intensive physicochemical effect in the soil. In this paper, a conceptual chemo-mechanical coupling model for unsaturated soils is proposed to explain the influence of pore fluid chemistry on the mechanical behavior of unsaturated clays. The intergranular stress is introduced as the constitutive variable that can effectively account for the physicochemical effect of osmosis, capillarity, and adsorption. The formulation of the model can lead to a remarkable unification of experimental results of tests carried out under complex chemical-mechanical loading conditions. The proposed model is validated by comparing the theoretical calculations with the experimental results, showing that the model is capable of addressing the effect of water content, concentration and species variation on the mechanical behavior of the clayey soil.

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A framework for integration of ‘gradation curve’ in the description of mechanical behaviour of unsaturated soils

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This paper presents a framework for incorporation of parameters relating to ‘Particle Size Distribution’ (PSD), or ‘gradation curve’ of soils in the constitutive description of unsaturated soils at low degrees of saturation. Unsaturated soils have ‘self-equilibrating’ initial stresses arising from surface tension forces acting on water menisci which depend on micro-structure of saturation and ‘Pore Size Distribution’ (POSD). The latter in turn can be related to PSD if simple shape of particles, spherical or elliptical is assumed. Assuming further, an idealised micro-structures of saturation in which both water and air phases of soil are continuous, a scenario corresponding to low degrees of saturation, it is shown how response of soils having same initial void ratio and the same degree of saturation is influenced by the gradation curve. In current approaches of modelling constitutive behaviour of unsaturated soils requires introduction of ‘Suction’ and ‘Soil Water Retention Characteristics (SWRC)’ as independent inputs, in a rather ad-hoc manner. In the proposed framework of description of mechanical behaviour of unsaturated soils, gradation curve of soil is adopted as an independent input. It is shown this to be a rational choice consistent with concepts of basic mechanics of soils. Numerical simulation of triaxial tests indicate qualitative agreement. However, there is a need for more controlled bespoke laboratory experiments to be conducted to check the validity and enhance the usefulness of the approach presented.

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A Model for Evolution of Soil Water Retention Curve with Void Ratio Using Energy Considerations

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A model for the evaluation of the Water Retention Curve (WRC) with void ratio is presented for deformable porous media. Current models in the literature are often phenomenological in nature requiring an extensive experimental program for parameter identification. The proposed model is however derived from energy considerations adopting the existence of generalized elastic and plastic potentials. Thus, it does not require any additional material parameter apart from the parameters specifying the WRC for the reference void ratio. The effects of hydraulic hysteresis and volume change dependency of the scanning curve are also incorporated in the present model. Furthermore, the model can gracefully capture the change in the hydraulic path of the sample from scanning to main and vice versa in a mechanical loading event. The applicability of the model to several experimental data from the literature is investigated. It is shown that the predictions of the volume change dependency of the WRC are in very good agreement with the published data.

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A model for retention curve in materials with evolving pore size distribution

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The retention curve (RC) has been historically considered as one of the constitutive laws required to close the water mass balance equation, together with Darcy's law and the state equation of water. As such, it is most commonly modelled by ad-hoc and one-to-one relationships between water potential and water content (or degree of saturation) and there exist in the literature many expressions to this purpose. Additional dependencies have been sometimes considered to capture hysteretic effect, always in the framework of the search for a functional relationship between hydraulic state variables.

More recently, the focus has been put on the strain dependency of the retention curve, and, more particularly on the strong link existing between RC and material pore size distribution (Durner, 1994; Romero & Simms, 2008; Casini et al., 2012). Besides the fact that water storage depends on pore network geometry through menisci distribution (Hassanizadeh, 2016), these works also help in putting forward the effect of the change in Pore Size distribution on the whole shape of the retention curve. As a consequence, on top of suction, straining can be shown to modify in quite complex way material water retention.

In this work, a model is presented to fully couple the retention curve to the mechanical response of the material. Proposed coupling is developed within a hydro-mechanical elastoplastic framework able to model simultaneously the hysteresis of the retention curve, the dependency of elastic parameter on suction through the definition of effective stress directly derived from the retention curve (Vaunat & Casini, 2016), the dependency of material limit envelope on degree of saturation and the change in the whole water retention curve under mechanical loading. The concept used for effective stress is first described and model framework formulated. Comparison with oedometer tests allow finally for a validation of the proposed bidirectional coupling between retention curve and material mechanical response.

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A new model for unsaturated expansive clays

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The constitutive modelling of highly swelling clays has been particularly challenging, despite significant recent efforts from the scientific community towards improving the modelling of unsaturated soils in general. One significant drive for this has been the application of such clays, bentonite in particular, in the design of engineered barrier systems in deep nuclear waste disposal. The existing constitutive models have difficulty in predicting with sufficient accuracy the effectiveness of sealing that the bentonite is expected to produce in order to protect the canisters in deep geological repositories.

The main features of a new double porosity structure model for unsaturated expansive clays are presented in this work, along with some details of its numerical implementation in a finite element code (Potts & Zdravkovic, 1999). Similar to the BExM (Barcelona Expansive Model; Gens & Alonso, 1992; Alonso et al., 1999; Sanchez et al., 2005), two structural levels are distinguished: macrostructure, groups of closely packed aggregates separated by macro-pores partly-filled with water, and microstructure, alternation of thin layers of clay and water that builds a single aggregate.

The model has a multi-dissipative framework and one of the plasticity mechanisms characterises the microstructure of the material, but also affects its overall behaviour. This is fundamental to the formulation as the peculiarly high swelling potential of these soils is physically explained through their mineralogical composition and fabric structure. Moreover, several studies have shown how this microstructure evolves upon loading and wetting. In particular transition from a double-structured to a single-structured fabric has been documented upon first wetting (Seiphoori et al., 2014).

The model considers the microstructure as always yielding: according to the total volumetric strain, micro-swelling or micro-contraction generate total plastic strains that are added to those of the macrostructure, which follows a BBM framework (Barcelona Basic Model; Alonso et al., 1990). Hence, the material evolves at both scales, in particular the hardening parameter of the microstructure is the microstructural void ratio, which is initialised as a fraction of the macro-structural one.

The model is numerically robust and some validation examples are presented. Although further development is foreseen, it is a priority to test this modelling approach in large-scale simulations, in order to further assess its predictive capability.

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Behaviour of suction within void ratio-moisture ratio-net stress space

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The relationship between the moisture level and soil suction is generally referred to as the soil water characteristic curve (SWCC) or the water retention curve (WRC). The soil moisture level may be represented by various parameters like gravimetric or volumetric water content or the degree of saturation. The gravimetric moisture content can also be presented as moisture ratio (given as volume of water divided by volume of solids, which is also equal to gravimetric moisture content multiplied by specific gravity). The relationship between soil moisture and suction is also dependent on the net stress level and (or) void ratio of the soil. In addition, hysteresis is generally present between drying and wetting parts of the SWCC curve giving primary wetting and drying curves. The shift from wetting to drying and vice versa is normally captured by what is known as scanning curves that connects the primary curves.

The present paper examines the behaviour of suction within void ratio-moisture ratio-net stress space. The data sets available in literature are analysed to examine these relationship in virgin compression states (on the compaction surface or loading wetting state boundary surface, LWSBS) and states unloaded to different net stress levels. In most cases, the suction is measured after compaction when the soil is fully unloaded. In this instance, suction is considered to correspond to unloaded states at nominal stress. However, some data are also available to examine the relationships of suction on the LWSBS and in unloaded states. These data are analysed to propose a hypothesis for SWCC in the form of moisture ratio versus suction and its dependency on net stress and void ratio. In the proposed paper, the main attention is paid to the primary wetting curves.

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Challenges of experimental and modelling hydro-chemo-mechanical mechanisms in porous chalk reservoirs during production operation

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Carbonate reservoir rocks are complex porous environment where several physical and chemical processes are coupled together forming a multi-physics and multi-phase system. Any attempt to simulate the system should consist of fundamental research on experimental and numerical aspects of the system. Intervening with the reservoirs, drilling and production operation, add another dimension to the simulation, behaviour over time. Therefore, some experiments and associated models should aim and consider the time effect. In the current study, rock mechanical tests were performed on chalk outcrops in a test bench coupling a hydro-mechanical system at elevated temperature with chemical feature of diverse flooding fluid ranging from simple brines to synthetic seawater. Typically, different mechanisms are coupled to different ions present in injecting fluid to the reservoirs. The role of each involved ion in chemically originated water weakening mechanisms is described. Magnesium and sulphate ions showed paramount contribution in changing the rock properties in term of wetting state and mechanical strength where sample treated with Magnesium/Sulphate ions presented weakly water-wet and weaker characteristics. The acquired data then is used to verify and validate first building block of a hydro-chemo-mechanical model. The parallel modelling work shows super saturated carbonate minerals in simulated environment similar to experiments environment. Validated model used to provide information on behaviour of chalk in more complex aqueous environments. All the experimental results and geochemical modelling pave the road toward building a chemo-mechanical model for carbonate rocks.

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Depressurization of heterogeneous aquifers and formation of anomalous transport: an experimental analysis

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The presence of connected structures affects the behavior of solute transport in heterogeneous aquifers. In particular it generates "anomalous transport", which characterizes the typically nonsymmetric breakthrough curves (BTCs) observed during tracer tests. These BTCs display pronounced “tailing”, which means longer-than-expected breakthrough of contaminants at a control section. According with the results of recent analytical, numerical and experimental studies, nearby pumping wells anomalous transport seems to be controlled by the impact of connectivity and stratification of flow and transport. While these conclusions were mainly drawn from the interpretation of flow and transport under saturated aquifer conditions, a new experimental investigation was conducted to evaluate the impact of connectivity on anomalous transport and scaling of BTCs under variably saturated aquifer conditions. Several experimental tracer tests were performed in a metric-scale heterogeneous sandbox from 26 different injection locations. Two sets of tests have been performed on the same sandbox with the same hydrogeological configuration. One set was performed under unsaturated settings (phreatic aquifer) and one set under fully saturated conditions (confined aquifer). In both sets, a pumping well at the center of the domain was imposed to generate an identical discharge rate. We show that despite the presence of the same connected features in the two systems, the conservative tracer injected in the unsaturated sandbox resulted in highly skewed BTCs when measured at the pumping well, while in the corresponding confined system most of the BTCs injected from the same locations were symmetric, showing no influence on anomalous transport generated by connected features. We observed that in the unsaturated setting, the vadose-zone-enhanced vertical flow due to the presence of free surface and large contrasts in hydraulic conductivity triggered by the desaturation of gravel channels nearby the pumping well which causes vertical mixing between gravel and sands, generating anomalous transport and BTC tailing. On the other hand, we observed almost negligible vertical mixing under saturated conditions and absence of anomalous transport. We conclude that in presence of fluctuating water tables (in our case induced by the presence of a pumping well) the lack of detection of anomalous transport from tracer tests under saturated conditions could generate misleading interpretations and predictions regarding the long-term fate of contaminants when saturation conditions are expected to change over time.

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Detailed Tests of the HYPROP Evaporation Method for Estimating the Unsaturated Soil Hydraulic Properties

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Many soil, hydrologic and environmental applications require information about the unsaturated soil hydraulic properties. The evaporation method has long been used for estimating the drying branches of the hydraulic functions. An increasingly popular version of the evaporation method is the semi-automated HYPROP© measurement system (HMinisymposium) commercialized by Decagon Devices (Pullman, WA, USA) and UMinisymposium AG (München, Germany). Several studies were previously carried to test the HMinisymposium methodology by using the Richards equation and the van-Genuchten-Mualem (VG) or Kosugi constitutive relationships to obtain synthetic date for use in the HMinisymposium analysis, and then to compare results against the original properties. We carried out independent tests of the HMinisymposium using the VG functions for a broad range of porous media. Our results closely agreed with previous findings. Accurate estimates were especially obtained for the soil water retention (Pc-S) curve and its parameters, at least over the range of available retention measurements. We also successfully tested a dual-porosity soil, as well as a medium with a very high van Genuchten n value reflecting a very narrow pore-size distribution (n=10). The latter case gave excellent results for water retention, but failed for the unsaturated hydraulic conductivity. In many cases, especially for soils with intermediate and high n parameter values, an independent estimate of the saturated hydraulic conductivity should be obtained. Overall, the HMinisymposium methodology performed extremely well and as such constitutes a much-needed addition to current unsaturated porous media hydraulic measurement techniques.

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Determination of fluid-fluid interfaces in unsaturated soils: the current key challenges

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Hassanizadeh and Gray (1993) suggested that the hysteresis in Pc-S (capillary pressure-saturation) relationship is due to neglecting a third state variable, namely, specific fluid-fluid interfacial area. Later on, Cheng et al. (2004) presented results of micro-model experiments which were indicating that inclusion of specific interfacial area can help modeling the hysteresis phenomenon. Apart from the hysteresis phenomenon, interfaces are the place of mass, momentum, and energy transfer, therefore, they are playing a significant role in the problems of environmental geotechnics where multiphase geo-materials are involved (Grant and Gerhard, 2007, Niessner and Hassanizadeh, 2009, Nikooee et al. 2013). However, the experimental and numerical determination of specific interfacial area is not an easy task. In this contribution, we summarize the key challenges in determining specific interfacial area based on the other state variables such as degree of saturation and matric suction (capillary pressure) and introduce some of the latest achievements.

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Effective stress versus elastic deformations: a numerical investigation

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Herein results from model systems of spherical beads (Fig. 1) with saturation ranging from 1 (saturated) to nearly 0 (pendular state) help revisiting a number of issues in relation with the concept effective stress and its generalization in partial saturation. The numerical experiments show that a micromechanical expression of the effective stress based on the averaging of solid contact forces (the Love-Weber (LW) averaging) appears as a rather good microscale counterpart of the effective stress in many cases, with respect to both the elastic deformation and the yield criterion. This result may sound intuitive but it is in fact a very intriguing feature of granular systems, and we offer a number of counter-examples in which this property breaks down. Namely, the elastic deformation in the pendular regime is not exactly controlled by the LW stress, and some special particle size distributions also cause it to loose relevance with respect to the yield criterion. Three general conclusions supported by the numerical experiments are: 1) there is no unique - ex-nihilo - expression of the effective stress, effectiveness necessarily refers to a particular constitutive relations (e.g. the elastic vs. the plastic effective stress in Coussy [5]); 2) the difference between the total stress and the effective stress is not a spherical tensor in general, the spherical approximation leads to serious inconsistencies; 3) the assumption of energy separation (according to which the elastic potential only depends on the effective deformation [5]) is violated in granular systems even for stiff grains.

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Effects of repeated hydraulic loads on the hydromechanical response of an unsaturated silty soil

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Soils used in earth constructions are mostly unsaturated, and they undergo frequent drying-wetting cycles due to seasonal changes in the climatic conditions (influencing the soil particularly at shallow depths) or due to changes in the water height of leeves and dykes. Changes in water content significantly influence the hydromechanical behaviour of the construction material, which therefore has to be assessed for repeated hydraulic loads. The research work here presented the coupled hydromechanical behaviour of a silt, typically used in the construction of dykes, with the aim of providing a better understanding of the consequences of drying-wetting cycles on the overall response of the material. Complementary laboratory tests were carried out to study the impact of drying-wetting cycles on microstructural features (provided by Mercury Intrusion Porosimetry and Environmental Scanning Electrical Microscopy analyses) and on the hydromechanical behaviour (oedometer and triaxial tests) of samples initially prepared by means of static compaction. The maximum contractive strains obtained upon drying were quite moderate, although they increased during the first two-three cycles, implying irreversible volume strains. During subsequent cycles, no increase in the volume strains was observed. As shown in Figure 1, the pore size distribution (PSD) of silt samples showed that repeated hydraulic loads changed the soil fabric by increasing the fraction of larger pores, which was different from fabric changes reported in the case of active clay (e.g. Romero et al., 2011). This microstructural evolution caused noticeable changes in the hydromechanical behaviour of compacted silt. As for the hydraulic response, samples subjected to 3 and 6 drying-wetting cycles had a reduced capacity to retain water than as-compacted samples. The permeability of such samples was higher than the one of the as-compacted samples over the whole saturation range (Figure 2), because the former have a more open fabric that leads to an easier path for water flow. The effects of repeated hydraulic loads on the mechanical behaviour were studied by means of triaxial tests. Isotropic compression at constant suction was imposed, followed by shearing at constant water content. Along isotropic compression, samples that had experienced drying-wetting cycles were more compressible than as-compacted ones, particularly at low-stress levels. As for shearing phase, such samples possessed lower void ratio and water content comparing to as-compacted ones, resulted in presenting higher strength and an increase in their tendency to dilate. Microstructural and macrostructural experimental evidences were interpreted in terms of a new approach which was developed based on the framework proposed by Della Vecchia et al. (2015). The proposed approach aims at accounting for the evolution of microstructure upon drying-wetting cycles. This allowed reproducing the effect of repeated hydraulic loads on water retention behavior, and on the mechanical behavior observed along the different generalized stress paths.

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Elasto-Plastic Behavior of an Unsaturated Compacted Non-Plastic Silt

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Response of unsaturated soils constitutes an important consideration for many problems in geotechnical engineering. A comprehensive laboratory-based study has been carried out to investigate the effects of matric suction on shear strength of compacted specimens; using a triaxial setup modified with axis translation for suction control, cell fluid volume measurement for monitoring specimen volume changes, and diffused air volume indicator for tracking the water content (Ahmadi-Naghadeh 2016). The results of a test programme on a non-plastic silt show that the shear strength of the studied soil increases nonlinearly as suction increases. The response of the specimens change from strain-hardening in saturated condition to strain-softening as suction increases. For the same net confining stress, specimens with higher suction values reach a peak deviator stress at lower axial strain. In general, total volumetric deformation behavior becomes more dilative as the suction increases. The laboratory test results were also interpreted under elasto-plastic framework for unsaturated soils and following conclusions were drawn: The critical state lines were generated through the results of the constant suction triaxial tests. The gradient of the critical state line, M, was determined for each test series. Consistent with Barcelona Basic Model (Alonso et al., 1990), the gradient of the critical state lines was found to be a constant value and independent of the suction (Fig.1). The intercept of critical state line, μ(s), was determined for each set of constant suction triaxial tests. Consistent with Wheeler and Sivakumar (1995), a nonlinear relationship between critical state line intercept μ(s) and matric suction were observed (Fig.2). Yield points were determined from saturated and unsaturated triaxial test results. The estimated yield values were employed to generate yield locus in deviator stress – mean stress plane for each suction value. No elliptical yield curve whose axes are parallel to the axes of stress was found to satisfactorily fit each series of constant suction yield points. This is postulated to agree with near-elliptical yield curves that have inclined axes (Fig.3), as suggested by (Cui and Delage 1996). The inclination of the yield locus can be attributed to inherent anisotropic nature of the one-dimensionally compacted specimens. It was found that, the size of the yield locus is suction dependent and expands as the suction increases. This observation is consistent with hardening effect of the suction, as included in Barcelona Basic Model by Alonso et al. (1990). The volumetric and deviatoric plastic strain increments were calculated to examine the flow rule. It was found that, for compacted specimens the associated flow rule (normality) was not satisfied (i.e. the plastic strain increment vectors were not perpendicular to yield locus).

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Elastoplasticity of unsaturated evolving porous media: application to cement paste hydration

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In order to adequately model the performance of cement-based materials, a holistic approach is required, integrating the progressive hydration of the material, the coupling between water consumption and strains, and the history of the applied loadings. This is particularly important for modelling the behavior of the cement sheath in oil wells which is subjected, from its earliest age and during its lifetime, to a wide range of mechanical and thermal loadings. Setting conditions such as pressure, temperature and subsequent loadings could have a detrimental effect on the future mechanical properties.

In the present work, the behavior of cement paste is described in the framework of reactive porous media. The cement paste is modelled as a multi-phase porous material with an elastoplastic constitutive law, with elastic and plastic parameters depending on function of the hydration degree. Furthermore, the pore water consumption during hydration and the cement chemical shrinkage are accounted for in the determination of the macroscopic shrinkage. The model contemplates the possibility of desaturation of the porous matrix as a result of water pressure drop due to hydration reaction and chemical shrinkage.

The model parameters for a class G cement paste are evaluated by simulating the results of mechanical loading experiments, performed using the STCA (Slurry To Cement Analyzer) in oedometric configuration. The STCA, conceived by TOTAL, is a device specially designed for testing the thermo-mechanical behavior of cement paste from the early stages of hydration. The macroscopic deformation of a cement paste sample is recorded continuously during hydration under constant axial stress and later on under loading-unloading cycles.

The evolution of the poroelastic parameters of the cement paste during hydration is calculated by means of a micromechanical upscaling model. A Drucker-Prager type yield surface with a cap and a non-associated flow rule are adopted for the elastoplastic regime, with hardening mechanisms considering both the cumulated plastic deformations and the hydration degree. A water retention curve is introduced to account for the potential desaturation of the material during hydration.

The results show that the proposed model predicts with good accuracy the response of a hydrating cement paste when subjected to various loading paths from its early age. The importance of the loading history is outlined, as well as the need for the accurate determination of the effective stresses in partially saturated conditions throughout the early age, especially for low-pressure curing conditions. Partial saturation is shown to have a significant effect on the effective loading path of the specimen.

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Evolution of the retention curve during expansion

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Different researchers have studied the effect of wetting on the pore size distribution on expansive soils. These results show that intra-pores largely increase their size and frequency while intra-pores reduce their size and frequency in such a way that they almost disappear. This means that intra-pores increase their size and volume and at the same time invade the inter-pores as the soil wets. This behavior has important repercussion on the retention curve. However experimental restrictions make it difficult to observe the evolution of the retention curve as the soil is expanding. The aim of this paper is to study the evolution of the retention curve for expansive materials as they wet. The study is based on a porous–solid model able to simulate the retention curve during wetting-drying cycles. The porous-solid model is based on the current pore size distribution of the soil and therefore, when the evolution of the last is known, it is possible to simulate the evolution of the retention curve as the soil wets.

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Experimental investigations on the role of transient effects within the drying-wetting behaviour of two different sands

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The relationship between moisture content, often expressed as degree of saturation, and the capillary pressure or matric suction in partially saturated porous media represents a key function as it can be used for the mechanical and hydraulic description and interpretation of the unsaturated porous medium. In soil mechanics this relationship is known as the soil-water characteristic curve (SWCC), because under natural conditions water and air represent the only liquid and gaseous phases which fill the pore space of a soil. Due to different hydraulic phenomena on the microscale the SWCC is highly nonlinear and also encounters hysteresis. This intrinsic relationship is in most cases determined and also modelled for unique equilibrium states between degree of saturation and capillary pressure by time consuming laboratory tests. Under natural conditions however, the equilibrium state will only rarely occur due to transient effects such as enforced flow conditions due to heavy rain or extensive evaporation.

In this contribution an experimental method is presented which allows to prescribe transient drying-wetting paths to small sand specimens, while the response of matric suction is measured in the middle of the specimen with a tensiometer. The centered tensiometer position in combination with the small specimen size and the assumption of a homogenised degree of saturation allow to combine the applied degree of saturation and measured suction to a macroscopic SWCC for the sand specimens. In the experiments different hydraulic flow rates of pore water can be applied to investigate their influence on the different obtained hydraulic paths of the SWCC. Furthermore, the tests allow to have a look at the nature of the obtained hydraulic paths for many transient hydraulic cycles and assess a possible drift in the curves as well as the effect of air entrapment.

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Micro-mechanical analysis of an effective stress variable for wet granular media

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Micro-mechanical modelling approaches are conducted in an attempt to identify a single-valued effective stress variable that would consistently govern the constitutive behaviour of both dry and unsaturated granular materials.

In a first step, an analytical stress homogenization approach separates the various stress contributions from the total stress of unsaturated granular materials. As a result, diverse stress contributions arise from contact forces between solid particles, fluid pressure within fluid volumes, and surface tension forces within the interfaces [1]. These stress contributions are microstructure-dependent, which leads to the fluid mixture stress contribution, often denoted as suction stress [2], to possibly include a deviatoric component, and thus deviate from an averaged (isotropic) fluid pressure.

In a second step, a Discrete Element Method (DEM) numerical model for wet granular materials [3] is used to assess the constitutive role of the various stress contributions. The DEM model applies to ideal granular materials with spherical particles, under very low wetting saturation in the so-called pendular regime. Accordingly, partially saturated conditions are described within the model by introducing distinct capillary bridges between particle pairs. The capillary bridge distribution is assumed to obey thermodynamic equilibrium and uniform capillary pressure conditions. As such, capillary bridges are readily computed by solving the Laplace-Young equation for given capillary pressure and contact angle values [3].

The DEM model provides a comprehensive access to the microstructure of all bulk phases and interfaces, including the various stress contributions. These are investigated in both loose and dense granular assemblies along different loading paths under dry and wet conditions.

As salient results of this study, the deviatoric character of the suction stress is first numerically demonstrated, highlighting the need to account for the material's microstructure for a proper stress assessment of unsaturated porous media [1,4]. Then, the nature of the stress contribution arising from contact forces between solid particles, and denoted as contact stress, is elucidated. In line with other recent results [3,5], the contact stress is shown to unify the failure description of dense and loose granular media under dry and wet conditions, provided that the solid phase packings are comparable. Furthermore, identical contact stress-strain paths are evidenced for both dry and wet materials. Such an equivalence is observed during the 'pseudo-elastic' regime of various loading paths (triaxial, oedometric) for which identical microstructural evolutions for the solid phase (average contact number, contact fabric anisotropy) are confirmed. Accordingly, the contact stress is shown to correspond to a single-valued effective stress variable for 'pseudo-elastic' behaviour description, and additionally, failure.

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On the role of nanoscopic disjoining stresses in the overall stiffness of expansive clays – a multi-scale approach

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In a former paper [1] we proposed a three-scale extension of Terzaghi's effective stress principle to unsaturated swelling clays that was rigorously derived by periodic homogenization starting from micro- and nano-mechanical analyses. The model derivation is based on a typical multi-scale representation of clay minerals characterized by three length-scales and two porosity levels:

• At the smallest nano-scale the medium is composed of incompressible clay platelets separated by a nano-porous network which is saturated by an electrolyte solution with completely dissolved ions giving rise to an electrical double layer (EDL); • At the intermediate micro-scale the clay platelets assemble to swollen clay particles building the compressible solid phase at that length-scale. The particles are separated by a micro-porous network filled by bulk water and air allowing to account for capillary pressure effects.

This model approach allows express the total stress at the observable macro-scale as the result of three terms: contact, capillary and disjoining stress contributions. In an application to numerically simulate the hydro-mechanical behavior of compacted bentonite during oedometric water infiltration tests we showed the ability of this multi-scale model to clearly identify the contributions of (microscopic) capillary and (nanoscopic) disjoining stresses to the overall swelling pressure over the entire water saturation range [2]. In addition, this numerical application points out that the medium stiffness might be ensured by the disjoining stress (originating from EDL and particle size effects) rather than by the clay platelet connectivity in order to recover the mechanical properties typically measured for clayey minerals.

The present work proposes thus an alternative formulation of the two-scale effective stress principle of the solid phase at the micro-scale allowing to include nanoscopic disjoining stress contribution in the clay particle stiffness.

The potential of this reformulation of the clay particle rigidity as a function of the disjoining pressure in capturing the impact of inter-platelet porosity and ion concentration on the mechanical properties of expansive clays is shown by numerical analyses.

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Pathway development and connectivity during gas injection / dissipation tests: Experimental results and numerical modelling

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Compacted bentonite-based materials have been used as engineered barriers in deep geological disposal of high level radioactive waste. The main purpose of these barriers is to delay the release of radionuclides and gases from the waste to the repository host rock. Therefore, it is essential to understand the gas migration process in compacted bentonites. Controlled volume-rate gas injection followed by dissipation stages have been performed under oedometer and isotropic stress conditions, which have been focused on the volume change response and the changes in the pore and pathway network Mercury intrusion porosimetry results have allowed detecting preferential pathways after gas injection / dissipation tests. The opening of these pressure-dependent pathways plays a major role on gas permeability. A complementary insight into the connectivity of these pathways has been quantified by micro-computed tomography (Voorn et al, 2013). Results have been used to estimate degree of saturation changes on gas injection due to the desaturation of the connected pathways. Numerical simulations using 2D axi-symmetric finite elements with CODE_BRIGHT have been carried out to model gas flow using a coupled hydro-mechanical model with stress dependent embedded pathways (Olivella & Alonso, 2008). The model handles the combined phenomena of two-phase flow (gas and liquid) and the aperture of discrete pathways to account for permeability and capillary pressure variations. Three zones with different material properties have been considered: a) central zone of pathway development; b) bentonite matrix; and c) upstream and downstream reservoirs to capture density of the pressurised air mass (Gonzalez-Blanco et al, 2016). The numerical results have reproduced upstream / downstream pressures, outflow volume and soil volume changes accurately. The combination of experimental results and numerical simulations have also provided a good insight into the role of the volume change response and pathway development on the gas transport properties of compacted bentonites, confirming that pathway development and aperture occurs during gas injection that later affects the response during the dissipation stage.

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Shrinkage Behavior and Correlation with Soil Water Retention under Self-Consolidation

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Soils show characteristic volume shrinkage as the volumetric water content decreases during drying under free external stress conditions. Traditional soil shrinkage curve (SSC) is divided into three phases: normal shrinkage when soil is saturated, residual shrinkage when soil is unsaturated, and zero shrinkage when soil approaches to dry state. By using drying cake technique, we simultaneously measured the volume changes, soil water retention (SWR) curves, and suction stress characteristic curves for various silty and clayey soils. A new SSC model was proposed associated with soil water retention regimes, and the volume reduction was re-interpreted by four states, i.e. capillary, pendular, adsorbed, and tightly adsorbed states. Each state is governed by one or/and two SWR mechanisms: capillarity and adsorption. The shrinkage rate, defined as the change in void ratio due to the change in moisture ratio, is not zero in adsorptive states. It is found that the shrinkage rate in adsorption SWR regime is highly related to SWR characteristics, i.e., specific surface area, cation exchange capacity, or maximum adsorption water content. The semi-logarithmic relation between void ratio and suction stress is defined as self-consolidation by environmental loading, i.e., drying or wetting. The isotropic compression index also presents strong linear correlation with the Atterberg limits for all soils. The soil shrinkage behavior under self-consolidation conditions connects the fundamental SWR characteristics with practical geotechnical index of soils through the deformation behavior, providing a potential new methodology to classify expansive soils.

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Shrinkage of concrete as an effect of hygro-mechanical coupling in unsaturated porous body – experimental and theoretical study of different poroelastic approaches

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Drying of cement-based materials, both due to evaporation from the surfaces and autogenous processes due to hydration of cement, lead to shrinkage and consequently often to cracking. In order to predict and mitigate shrinkage, a proper understanding of its mechanisms and key parameters is necessary. In this work, we apply different poroelastic approaches to predict autogenous and drying shrinkage of cement-based materials. The theoretical study is presented together with experimental data on shrinkage of cement paste and mortars. The study focuses in particular on the discussion of the effect of saturation on the predicted strains. It is shown that in materials with pore sizes ranging from nanometers to micrometers, the determination of saturation degree, and consequently the shrinkage predictions, are affected by some arbitrary assumptions regarding the reference (dry) state. A further topic discussed in the presentation is the presence of a visco-elastic component in the shrinkage strains and its importance in shrinkage, restraint stresses and cracking predictions.

Figure: Prediction of drying shrinkage of w/c 0.50 mortar with Biot-Bishop model [1]

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Transient Hydration of Compacted Bentonite Based Buffer Material in Under Ground Disposal of Nuclear Waste: Challenges and Experimental Investigations

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In recent years, considerable research has been carried out to characterize the compacted clay based buffer material in the frame of coupled thermo-hydro-mechanical (THM) processes at nuclear waste repositories. In this context, initially unsaturated buffer is subjected to radioactive decay heat emitted by waste canister in conjunction with peripheral hydration through host rock. Montmorillonite based clay minerals - water interaction induces significant expansion of stacked clay layers on micro level and exerts swelling pressure. Soil water retention and swelling mechanism are dependent on applied volume constraint condition. In repositories, volume constraint conditions evolve in transient manner from initial free swell condition to swell under constant volume condition due to available technological voids. The technological voids are referred to as the macro-pores related to different interfaces involving the buffer material. One of the major challenges is to anticipate the material behaviour under such transient boundary conditions. Dual porosity based constitutive models are well suited for explaining the soil water retention behaviour of compacted clays. Enhancement of existing dual porosity models requires incorporating the inputs regarding clay microstructure and its evolution from phenomenological investigations identical to the actual one. The errors associated with element tests due to scale effect, steady state boundary conditions and lack of generating repository relevant loading scenarios can be eliminated in phenomenological experiments. In this connection, a unique column experiment device is designed as a forerunner of field scale test at Ruhr Universität Bochum to simulate the transient hydration process of compacted buffer under repository relevant boundary conditions. The device is unique in terms of having proficiency to capture the transient material response under various possible repository relevant loading paths with higher precision level by monitor the key parameters like temperature, soil total suction, water content and axial and radial swelling pressure at three different sections along the total length of 30 cm. In general, a larger spectrum of loading paths / scenarios, which may arise in the nuclear repository, can be covered precisely with this devise. The initial test results are also reported in this paper as a part of device validation and calibration studies.

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Wetting collapse of a unsaturated pyroclastic soil: constitutive modelling

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The Pastor-Zienkiewicz model is suitable to describe the behaviour of loose or dense granular soils, in drained and undrained conditions, even along complex stress paths. This framework was recently extended by to the case of unsaturated sands subjected to large variations of both relative density (Dr) and confining pressure (p'), through the introduction of a state parameter, which measures the difference between the current void ratio and the critical void ratio at the same mean effective pressure.

In this paper, the modified Pastor-Zienkiewicz model (MPZ) is applied to the case of an unsaturated air-fall volcanic (pyroclastic) soil of Southern Italy, originated from the explosive activity of the Somma-Vesuvius. A series of wetting tests, performed on undisturbed specimens in oedometric and triaxial conditions, were simulated. Indeed, the so-called wetting collapse is one of the most common problems associated with unsaturated soils, causing huge slope stability problems and catastrophic consequence in the case of flow-like landslides.

The results achieved show a satisfactory capability of the MPZ to simulate the volumetric strain experienced by all the specimens after the wetting path. The possible modelling improvements are also outlined.

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X-ray Computed Tomography investigation of unsaturated pyroclastic soils upon wetting

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The X-ray Computed Tomography (CT) allows recording a set of radiographies of a soil specimen at different angular positions and the reconstruction of 3D image of each single solid grain, voids among grains and water filling the voids. This advanced experimental technique was used to investigate the modifications of the internal structure of two unsaturated sands upon wetting. The investigated soils were derived by a natural volcanic (air-fall) pyroclastic soil of Southern Italy, characterised by an open metastable structure due to air-fall origin, and frequently involved in flow-like landslides. One of the relevant mechanisms is the so-called wetting collapse, formerly studied at macroscopic scale by several authors and through many different devices at Representative Elementary Volume (REV) scale. The aims of this micro scale experimental investigation were to: i) follow the transformation of the specimen's microstructure; ii) evaluate the variation in terms of water content, porosity and grains spatial distribution; iii) analyze the effect of grain size distribution on the development of capillary forces and mass forces. The tests were carried out on both fine and coarse sand. During the test, the specimen was subjected to its self-weight and no stress was applied, while the suction was gradually reduced until the complete collapse occurs. It was measured that the collapse is obtained at a certain threshold in suction and it is not mandatory to reach the complete saturation.

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4D XMT of Reaction in Carbonates: Reactive Transport Dynamics at Multiples Scales

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Upscaling pore scale rock-fluid interaction processes for predictive modelling poses a challenge to underground carbon storage. We have completed experiments and flow modelling to investigate the impact of pore-space heterogeneity and scale on the dissolution of two limestones at both the mm and cm scales. Two samples were reacted with reservoir condition CO2-saturated brine at both scales and scanned dynamically as dissolution took place. First, 1-cm long 4-mm diameter micro cores were scanned during reactive flow at a 4-µm resolution between 4 and 40 times using 4D X-ray micro-tomography over the course of 1.5 hours using a laboratory µ-CT. Second, 3.8-cm diameter, 8-cm long macro cores were reacted at the same conditions inside a reservoir condition flow rig and imaged using a medical CT scanner. Each sample was imaged ~10 times over the course of 1.5 hours at a 250 x 250 x 500-µm resolution. The reacted macro cores were then scanned inside a µ-CT at a 27-µm resolution to assess the alteration in pore-scale reaction-induced heterogeneity. It was found that both limestones showed channel formation at the pore-scale and progressive high porosity pathway dissolution at the core-scale with the more heterogeneous rock having dissolution progressing along direction of flow more quickly. Additionally, upon analysis of the high-resolution macro core images it was found that the dissolution pathways contained a distinct microstructure that was not visible at the resolution of the medical CT, where the reactive fluid had not completely dissolved the internal pore-structure. Flow was modelled in connected pathways, the flow streamlines were traced and streamline density for each voxel was calculated. It was found that the streamline density was highest in the most well-connected pathways and that density increased with increasing heterogeneity as the number of connected pathways decreased and flow was consolidated along fewer pathways. This work represents the first study of scale dependency using reservoir condition 4D X-ray tomography and provides insight into the mechanisms that control local reaction rates at multiple scales.

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A generic transport-reactive model for simulating microbially influenced mineral precipitation in porous media

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Corrosion is a significant economic problem - recent reports evaluate the annual cost of metal corrosion as 3-4% of the gross domestic product (GDP), in both developed and developing countries. Corrosion control methods currently used are costly and unsustainable as they require the use of larger volumes of materials, hazardous chemicals and regular inspections. As an alternative corrosion control method, bioinfluenced deposition of protective mineral layers has been proposed. In the vicinity of corroding metal in soil a variety of precipitated natural crusts are observed. The blockage of pores by iron precipitates contributes to corrosion rate reduction in soils. Bioinfluenced precipitation of calcite has already been investigated for CO2 geological sequestration and soil improvement. However, controlling and quantifying the formation and properties of these crusts remains a challenge.

In order to improve our understanding of the processes that control (bioinfluenced) mineralization in porous media we conducted double-diffusion experiments using an agar and sintered glass filters as artificial soil. Chemical species are allowed to diffuse from both sides of the experimental tubes. The counter-diffusion of these species leads to precipitation of a mineral in the samples. The amount and distribution of precipitates are measured using a CT scanner and the permeability of the sintered glass samples is measured using the falling-head method before and after precipitation process. The distribution of the precipitates is in non-uniform, non-symmetric precipitation bands.

Our experiments generated unique data sets, that allowed us to calibrate and verify our mechanistic numerical model of (bioinfluenced) mineralization in soil. The numerical model includes three phases - solid, biofilm and water. The model is on REV scale, so that the properties are averaged over multiple pores. Mechanisms included are the physical transport of dissolved solutes, consumption of substrate and expulsion of metabolism products by the biota, chemical equilibrium reactions in the pore water and kinetic precipitation reactions. Changes in porosity and permeability of the porous medium through biofilm growth and solids precipitation are simulated.

We demonstrate how (bio)chemical changes in the pore water lead to changes in porosity and permeability. Data produced with our model, after calibration, are in good agreement with the experimental data. In addition, we show with several modeled scenarios that, by modifying soil conditions it is possible to control the precipitation zone - its rate of formation, location and density. This opens opportunities for engineering naturally deposited corrosion barriers in soils. However, even our relatively simple model involves complex interactions and numerous assumptions. Further numerical and physical experiments are needed to extend our understanding of the processes involved and the possibilities of “employing” micro-organisms to control the properties of the porous media.

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A pore-scale evaluation of bacterial mediated transformation of toxic Cr (VI) to Cr (III) by using real-time electrical capacitance method

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Bacteria-contaminant interactions in subsurface environment are deemed to have greater significance in remediation of heavy metal-contaminated aquifers. For a successful bioremediation, an approximate prediction on the bacterial interaction at pore-level must be known. Although there have been enormous laboratory studies focused on biotransformation of toxic contaminant Cr (VI) [1], much remains to be dealt with the pore-scale understanding of fate and transport of tolerant bacteria in the presence of the hexavalent chromium. The bacterial fate and transport in porous media involves the complex framework of biological processes such as growth pattern by adhesion, detachment, and chemotactic response during the presence of contaminant Cr (VI), which are governed by many environmental factors including nature of the geological strata, its heterogeneity and bioavailability of contaminant to the bacterial species [2] & [3]. Considering the major role of bacterial–contaminant interaction in real time subsurface environment, the present research attempts to show the pore-scale understanding of the bacterial mediated transformation of toxic Cr (VI) to Cr (III) by using Real Time Electrical Capacitance Method. A prior investigation on bacterial mediated reduction of Cr (VI) was conducted by using the isolates from chromium contaminated soil site. This procedure involves the isolation and identification of the species that actively take part in biotransformation. Column transport experiments were performed by allowing the tolerant bacterial species to react with toxic Cr (VI) under varying conditions; to record the real time changes in growth pattern along with their sorption characteristics by continuously measuring the electrical impedance. The Electrical Capacitance Method employed in this research work proves to be a promising non-intrusive real time approach to provide qualitative and quantitative three-dimensional image based information on bacterial fate and transport during the biotransformation of Cr (VI) to Cr (III). The consideration of real time bacterial behavior in the present study will provide a framework of pore-level modeling of Cr (VI) fate and transport, as a part of biogeochemical reactions in subsurface environment. Furthermore, it is expected that this real time monitoring technique can also provide insights into the various phase interactions of multi-phase flow system in depicting the complex transport phenomena in subsurface environment [4].

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A scalable, modular pore network model.

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Pore network models (PNM) are nowadays widely used as an investigative and upscaling tool in geoscience, most likely on account of their relatively low computational cost, that allows to simulate larger (and presumably representative) volumes of porous medium. Provided they are built on a topologically and geometrically sound basis, they have achieved predictability regarding flow [1]. Work is still under way to eliminate the most unrealistic assumptions (perfect mixing, Taylor-Aris dispersion) that allow simple (i.e. computationally cheap) modeling of the transport of solute, with the inevitable downside of increasing the computational cost [2]. Adding chemical reactions to the transport is the next logical, desirable step, even though it will further, drastically increase the computational cost. [3] These considerations have led us to develop a scalable, modular PNM software, to serve as a platform able to integrate existing and future models. Scalability is achieved through a complete parallelisation of the code, using MPI for inter-process communications and PETSc for linear algebra. The size of the PNM is thus only limited by the number of computers the program runs on. The topology and geometry of the network is constrained by user-supplied statistics (pore size, coordination number, etc.), on an ordered or random lattice. Physico-chemical processes are implemented as self-contained, possibly inter-dependent modules encapsulating the data and functions relevant to their model. They can be freely attached to, and detached from, the network. For reasons of performance, maintainability and expressiveness, the code is written in (modern) C++. We expose the challenges of the parallelization of PNM, show that its side-effects on the results are nonexistent or negligible, and present the opportunities it offers regarding flow, transport and drying [4].

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Absolute Permeability Estimation Using Smoothed Particle Hydrodynamics

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Smoothed Particle Hydrodynamics (SPH) method has found many practical applications since its original development for astrophysical flows (Gingold and Monaghan, 1977; Lucy, 1977), such as modeling miscible flows, surface tension and contact angles, unsaturated flow, reactive transport and precipitation (Tartakovsky et al., 2015). With a few exceptions (Holmes et al., 2015), SPH has been largely used to model two-dimensional problems in porous media studies (Tartakovsky et al., 2007).

We present a methodology to estimate absolute permeability in mm-size three-dimensional micro-tomography (u-CT) images of pore space using the SPH method. Firstly, we validate the method on a Poiseuille flow in an infinite parallel-plate geometry and Sod's shock tube problem. Next, we study and compare flow fields and permeability in three types of sphere pack arrangements: cubic, rhombic and loose random pack. Finally, the method is applied to look into the flow characteristics in a u-CT image of a Ketton limestone. With the increase of pore-scale complexity, that is from Poiseuille flow, through beadpacks to Ketton limestone, we observe more heterogeneous flow fields. Direct simulation provides a detailed information on sub-pore scale flow which is essential for accurate estimates of the macroscopic parameters. Our methodology serves a s a robust starting point in expanding our studies to more complex reactive and solid transport behaviour that we are developing using a coupled SPH and DEM simulator.

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An integrated pore scale and continuum scale study for solute dispersivity in a large-scale-saturated soil column

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In this study, we have combined 36-cm column experiments, X-ray 3D imaging, and pore network modelling of a large-scale experiment to explore solute dispersivity. Laboratory column experiments were carried out to obtain solute breakthrough curves (BTCs) at several longitudinal locations and to calculate solute dispersivity values along the sample and for different flow velocities. We have used X-ray imaging to extract a representative pore structure of the sample to build up a 36-cm long pore network model, allowing direct comparison of the pore-scale model to the experimental observations. Solute dispersivity was found to increase with length at a rate which is lower for higher applied velocity values. The statistically equivalent pore network model was able to simulate the measured BTCs. This provides confidence that this pore-scale approach can ultimately be applied to model the spreading of solutes at laboratory length scales.

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Apparent oil permeability in shale reservoirs considering the compressibility of porous media effect

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Shale oil reservoirs have abound micro-and nano-porous media, including kerogen and inorganic matrix. Compressibility has a great influence on changing the space and surface areas of micro-and nano-pores, which is of great significance to the gas transport mechanisms. In this paper we introduce a new mathematical apparent oil permeability formula to predict the volumetric flux of oil in shale reservoirs. In this formula, the effect of slip condition, pore shape, oil desorption are considered. Based on this, corrections to structure of shale (distribution of pore size, pore shape etc.) are made to properly model liquid flow in representation elementary volume (REV) of shale. Then, the changing regularity of pore size and surface area in REV with the compressibility will be discussed. Meanwhile some key parameters for liquid flow in shale reservoirs, including slippage factor, desorption coefficient, and other correction factors are analyzed considering the influence of the compressibility. Therefore, a fully coupled apparent permeability model are developed to describe liquid flow in shale. The proposed permeability expression is validated with an existing set of experimental data. The influence of compressibility on apparent oil permeability are analyzed with different pore shape, pore sizes and slippage condition. The model results show that the compressibility has a greater influence on the mean of pores within inorganic matrix than within kerogen. The model results also confirm that the apparent permeability is more sensitive to pressure change in inorganic matrix than kerogen. Finally, the influence of pore structure on apparent permeability are discussed. This work is important and timely for development of shale reservoir-flow simulators.

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Direct numerical simulation of pore-scale solute transport in three-dimensional porous media

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"In the present work, fluid flow and solute transport through sphere packing are described by solving the governing equations (the full Navier-Stokes equations) at the pore scale with finite-volume discretization. The three-dimensional sphere packings are created using DEM. Care is taken to evaluate numerical issues related to mesh generation, spatial discretization and domain size. The calculations performed are then examined though resulting velocity distributions and solute dispersion behaviour. Pore-network modelling of the same geometries are also attempted and results from both methods are compared and analysed."

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Experimental characterization of mixing dynamics in porous micromodels

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Mixing interfaces play a fundamental role in subsurface reactive processes by creating highly reactive localized hotspots of chemical and microbiological activity [1,2]. In many cases, the local reactivityis limited by the mixing dynamics which enables reactants to come in contact with each other[3].How the mixing dynamics depend on the relative magnitudes of advection and molecular diffusion, and how that dynamics is controlled by the geometry of the advecting velocity field,arecrucialquestions in this context. Recent studies have evidenced the role of stretched lamellae of solute whose rates of diffusive smoothing build up the overall mixture concentration distribution[4,5]. Here we present an experimental characterization of thetransport of a fluorescent solute inside amodel porous medium. Wemeasure the concentration field throughout the porous medium,as well as Lagrangian velocities along fluid particle trajectories, and characterize the mixingdynamics in terms of the concentration gradient distributionandcharacteristic mixing time,as a function of the Péclet numberand for different pore geometries. The measurements are consistent with recent theoretical predictions[4,5]which provide the link between the advecting fluid velocities and the concentration gradient of a transported solute.

Fig1:Visualisation of concentration gradients in a model 2D porous medium

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Exploring unsaturated colloid deposition and mobilization in 3D with x-ray microtomography

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Understanding the mechanisms controlling colloid transport and deposition in the vadose zone is an important step in protecting our water resources. Not only may these particles themselves be undesirable contaminants, but they can also aid in the transport of smaller, molecular-scale contaminants by chemical attachment. In this research, we examined the influence that air-water interfaces (AWI) and air-water-solid contact lines (AWS) have on colloid deposition and mobilization in three-dimensional systems. We used x-ray microtomography to visualize the transport of hydrophobic colloids as they move through a partially saturated glass bead pack. Both air-water, and air-decane systems were investigated to explore the effect of surface interactions on mobilization. Drainage and imbibition experiments were conducted using syringe pumps to control the flow of a colloid suspension through the porous media at 0.5, 5 and 50 mL/hr. During drainage, the flow was periodically halted and allowed to equilibrate before collecting the microtomography scans. Dopants were used to enhance the contrast between the four phases (water, air, beads, and colloids), including potassium iodide dissolved in the water, iodobenzene in the decane, and an outer layer of silver coating the colloids. We hypothesized that AWIs and AWSs will scour and mobilize a significant percentage of colloids, and therefore reduce the concentration of colloids along the vertical profile of the column.

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Flow in Coal Seams: An Unconventional Challenge

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A significant unconventional resource for energy is the methane gas stored in shallow coal beds, known as coal seam gas. An integrated imaging and modelling framework is developed for analyzing petrophysical behavior of coals. X-ray micro-computed tomography (micro-CT) is applied using a novel contrast agent method for visualizing micrometer-sized fractures in coal. The technique allows for the visualization of coal features not visible with conventional imaging methods. A Late Permian medium volatile bituminous coal from Moura Coal Mine (Queensland, Australia) is imaged and the resulting three-dimensional coal fracture system is extracted for fluid flow simulations. The results demonstrate a direct relationship between coal lithotype and permeability. Scanning electron microscope and energy dispersive spectrometry (SEM-EDS) together with X-ray diffraction (XRD) methods are used for identifying mineral matters at high resolution. SEM high-resolution images are also used to calibrate the micro-CT images and measure the exact aperture size of fractures. This leads to a more accurate estimation of permeability using micro-CT images. To study the significance of geometry and topology of the fracture system, a fracture reconstruction method based on statistical properties of coal is also developed. The network properties including the frequency, aperture size distribution, length, and spacing of the imaged coal fracture system. This allows for a sensitivity analysis on the effects that coal fracture topology and geometry has on coal petrophysical properties. A combined numerical and experimental approach is applied to obtain relative permeability curves for different regions of interest. A number of challenges associated with coal samples are discussed and insights are provided for better understanding of these complex porous media systems.

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Moisture absorption by salt confined in 2D porous media

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Hygroscopic salts are commonly present in porous materials used for the construction of buildings and outdoor sculptures. With fluctuations of the relative humidity in air, the entrapped hygroscopic salts can capture the moisture in the air and form a salt solution within the porous network. This process is known as salt deliquescence and starts when the relative humidity exceeds the equilibrium relative humidity above a saturated solution of the same salt. The formation of salt solutions can make that masonry, sculptures etc. become moist which can lead to deterioration. Upon subsequent drying, the crystallisation of the salt can cause weathering and can damage e.g. frescoes on their surface. We investigate the deliquescence of sodium chloride crystals entrapped in new model 2D porous media. A novel technique of fabrication of 2D porous media allows to create a system with well-defined properties; we create e.g. a bimodal pore size distribution and control the porosity and the location of entrapped salt. The 2D nature of our system allows to study the kinetics of the solid to solution phase transition of the salt by deliquescence and the fluid transport at the pore scale in a controlled mini-climatic chamber using a microscope. The rate of deliquescence and the volume increase of the brine solution within the porous network in time are measured by continuously imaging using a CCD camera. Our results show that the kinetics of deliquescence has three different regimes with a different time dependence of the increase of the liquid volume in the porous network. We also show that the subsequent invasion of the liquid in the porous network is controlled by the pore sizes and wetting properties of the porous network. For a hydrophilic medium, the liquid invades the small pores towards the exit of the porous medium whereas, in the hydrophobic system the salt solution preferentially invades the large pores. This can be explained by the difference in the capillary pressure between these two porous networks which depends on the contact angle and the pore size. After complete deliquescence, the drying of the solution in the hydrophilic system induces the displacement of the salt crystal from large pores towards the smaller ones. In addition, the crystals move towards the exit of the porous medium, showing a tendency to provoke efflorescence. For the hydrophobic system, the drying is exactly the reverse process of the deliquescence; the salt recrystallizes in the same pore where the initial crystal was located before the deliquescence started. The kinetics of deliquescence is modelled using a pore network model with characteristics of the 2D model network used in experiments. The model describes the experimental results well and allows for more insight into the dynamics of moisture absorption in porous media.

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Moisture distribution in the pore system of hardened cement paste: Implications on gas transport

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Cementitious materials are an essential part of the engineered barrier system (EBS) in nuclear waste repositories in which they are used as backfill and buffer material. Within a geological time frame the EBS can be subjected to the evolution of substantial amounts of free gas potentially jeopardizing the long-term safety of the system. Currently, a classic visco-capillary two-phase flow mechanism for the simultaneous transport of gas and pore water is assumed for which a profound knowledge of processes and influencing parameters is indispensable. In a capillary-controlled system like the EBS the saturation and the distribution of the wetting phase in the pore system have a crucial influence on the effective gas transport and effective migration pathways. Studying the water distribution in relation to the pore structure and other potentially controlling parameters is therefore of great interest and might have a tremendous impact on the interpretation and modelling of transport processes as well as related phenomena when transferred into application. This contribution reveals the preliminarily outcomes and experimental approach of a systematic study of water saturation as well as its distribution and in long-term its relation to and influence on gas permeability in cement-based materials.

To systematically study the water distribution, occupied pore sizes and governing parameters in the pore system of cementitious materials, high-resolution water sorption isotherms (303 K) were measured by means of dynamic vapour sorption using a gravimetric device. While the sample material (water-to-cement ratio: 0.4 to 0.5) was cured (28 days), the setup was calibrated via the deliquescence points of seven saturated salt solutions between 11 and 98 % relative humidity. The isothermal mass uptake (0 to 98 %RH) was measured on approximately 50 mg of gently crushed and dried bulk material at 303 K in ad- and desorption mode. Mineralogical representativeness was ensured by quantitative X-Ray diffraction analysis, while total porosity was determined on intact sample plugs via helium pycnometry. Additionally, nitrogen physisorption isotherm measurements were performed (77.3 K) on dry and moisture-equilibrated samples by a static-volumetric method. In the near future, the study will be extended by the application of µCT in order to approach the visualisation of gas flow in the pore network of hardened cement paste. The obtained results will contribute to the understanding of moisture distribution and sorption mechanism in the pore system of cementitious materials. Furthermore, on a long-term, the anticipated outcomes will be applied to experimentally investigate the relationship between gas permeability (dry and partially saturated samples) and water sorption hysteresis which, intuitively, should be reflected in the gas permeability due to a variation in saturation (Chen et al., 2012). However, this implies that the

transporting pore size contributes to or is affected by the hysteric behaviour of water which may be deduced from the current study.

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Multiscale Characterization of a Mixed Wet Carbonate using X-ray microscopy. Extending pore scale techniques to the whole core scale.

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Fluid flow in porous media is dominated by processes occurring at the scale of the microscopic tortuous pathways through the fluid flows and in which the fluids are hosted. The last 20 years have seen a step change in our ability to characterize and examine such flow at the scale at which these physical processes occur, with pore scale imaging and modelling being transformed from a primarily academic pursuit used to examine fundamental processes associated with transport and displacement to a fully-fledged industrial service industry, routinely used to by the oil industry to predict flow and transport properties of subsurface samples1. While many advances have been made, significant challenges remain, particularly in the areas of process and scale. Frequently subsurface flow is governed by multiphysical processes which are poorly understood and parameterized in real systems. We can begin to address this “problem of process” by using recent technological advances to examine multiphase flow processes experimentally in situ at the pore scale2,3,4. The second principal challenge is that of scale; while techniques exist with sufficient resolution to image fundamental pore structures in a wide range of different systems, frequently this comes at the expense of true subsurface heterogeneity5. As such, multiscale techniques must be developed to properly characterize this heterogeneity at a representative scale and then drive higher resolution characterization techniques. In this study we will show how these two challenges can be addressed together in the characterization of wettability distribution in a mixed wet carbonate sample. A 4” whole core sample of a heterogeneous carbonate was first imaged at low resolutions (33µm voxel size) across its entire width using a large field of view Flat Panel detector in the Zeiss Versa X-ray microscope. This initial scan showed prominent heterogeneity on the cm length scale. This heterogeneity was quantitatively characterized by classifying the low resolution image into different petrophysical units by local porosity. This macroscopic classification was used to drive the high resolution coring of the sample, deriving 5mm cores from the both the high and low porosity lithologies. These samples were then mounted into an in situ flow apparatus within the X-ray microscope, enabling for fluid flow experiments to be conducted on each sample. The samples were first vacuum saturated with brine, before the injection of both oil (drainage) and chase brine (imbibition) to establish a residual state, which was then imaged at intermediate (5µm) resolution. These images were then analyzed to locate the three phase contact line, which was then imaged again at high (2µm) resolution. These high resolution images were then used to measure local spatially resolved wettability using the technique outlined in Andrew et al.6, showing that the high porosity lithology was oil wet, whereas the low porosity lithology was water wet. Such heterogeneity of behavior can only be understood in the context of the macroscopic lithological heterogeneity of the sample. As heterogeneity was used to drive high resolution sampling, the resulting high resolution behavior can be upscaled back to the whole core scale much more readily, enabling for the first time both pore scale and core scale information to be integrated and analyzed concurrently.

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Multiscale lattice Boltzmann modelling of transport properties in porous media.

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The flow characteristics of heterogeneous rocks, such as carbonates and clay rich sandstones, are intimately tied to depositional and diagenetic processes. These complex pore structures, involving many orders of magnitude in length scales, cannot be captured by a single resolution micro-CT image. In the present work, a coherent multiscale workflow to calculate absolute permeabilities in heterogeneous rocks is developed. A dry/wet micro-CT imaging sequence provides a spatial mapping of porosity and connectivity in macro- and micro-porous regions. The registered 3D porosity map is then used as input to a gray-scale Lattice Boltzmann model. The model employs a partial bounce back scheme to mimic the resistance to flow in micro-porous regions. The bounce back probability in each lattice node is a function of partially resolved grain matter and local micro-porous phase permeabilities. The partial resolved grain content in each voxel is first estimated from porosity map information. The micro-porous phase permeabilities are then estimated through porosity-permeability relationships derived from 3D particle models based on nano-scale BSE images of each micro-porous phase. This new methodology is validated by comparing with known analytical solutions and high resolution models where the pore structures are completely resolved. Finally, experimental and numerical results are compared for several carbonate and sandstone samples.

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Multiscale Modelling of Dual-Porosity Porous Media; A Computational Pore-Scale Study for Solute Transport

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A large number of environmental and agricultural applications involve the transport of water and dissolved constituents through aggregated soil profiles, or in porous media that are structured, fractured or macroporous in other ways. During the past several decades, various process-based macroscopic models have been used to simulate solute transport in such media. Many of these models consider advective-dispersive transport through relatively large inter-aggregate pores, while exchange with the smaller intra-aggregate pores is assumed to be controlled by diffusion. Exchange of solute between the two regions is often represented using a first-order mass transfer coefficient, which is commonly obtained by fitting to the observed data. This study aims to understand and quantify the solute exchange term by applying a dual-porosity pore-scale network model for relatively large domains, and analyzing the pore-scale results in terms of the classical dual-porosity (mobile-immobile) transport formulation. We examined the effects of both aggregate porosity and aggregate permeability on the dual-porosity model parameters, being the relative amount of mobile water (φm) and the mass transfer coefficient (α). Results were obtained for a wide range of aggregate porosities (between 0.082 and 0.700) and the effects of aggregate permeability was explored by varying pore throat sizes within the aggregates. Solute breakthrough curves (BTCs) obtained with the pore-scale network model at several locations along the domain were analyzed using analytical solutions of the dual-porosity model to obtain estimates of φm and α. An increase in aggregate porosity was found to increase both φm and α, leading to considerable tailing in the BTCs. Changes in aggregate pore throat size affected the relative flow velocity between the intra- and inter-aggregate domain. Higher flow velocities within the aggregates caused a change in the transport regime from diffusion dominated to more advection dominated. This change increased the exchange rate of solutes between the mobile and immobile domains, with a related increase in the value of the mass transfer coefficient and less tailing in the BTCs.

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On the upscaling of the velocity in a slowly drying porous medium from pore network simulations

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We study the velocity field in the liquid phase during the drying of a porous medium in the capillarity-dominated regime with evaporation from the top surface. A simple mass balance in the continuum framework leads to a linear variation of the filtration velocity across the sample. By contrast, the instantaneous slice-averaged velocity field determined from pore network simulations leads to step velocity profiles. The vertical velocity profile is almost constant near the evaporative top surface and zero close to the bottom of the sample. The relative extent of the two regions with constant velocity is dictated by the position of the most unstable meniscus. It is shown that the continuum and pore network results can be reconciled by averaging the velocity field obtained from the pore network simulations over time. This opens up interesting prospects regarding the transport of dissolved species during drying. Also, the study reveals the existence of an edge effect, which is not taken into account in the classical continuum models of drying.

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Pore-scale investigations into the stability of residual CO2

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Despite its major influence on storage capacity, CO2 plume migration rate, and rates of CO2 dissolution and mineralization, residual trapping remains perhaps the least understood of the trapping mechanisms following CO2 injection in geologic formations. Although classical models of residual trapping assume that the disconnected ganglia of supercritical CO2 (scCO2), once pore-scale snap-off occurs, are permanently immobilized, potential phenomena such as further dissolution in brine, wettability alteration or Ostwald ripening, could lead to remobilization of residually trapped CO2.

The aim of this work is to investigate the permanence of residual trapping by i) assessing the potential for Ostwald ripening in rocks to remobilize trapped CO2 using synchrotron X-ray microtomography (micro-CT) analysis of pore-scale capillary pressure and modeling of Ostwald ripening mechanism in rocks, and ii) observing the stability of residually trapped scCO2 during the early stages following imbibition CO2 in a sandstone by conducting a drainage-imbibition experiment with reservoir conditions and time-resolved micro-CT imaging .

The results from the first experiment show that disconnected gas ganglia may present noticeably different capillary pressures and, as a result, Ostwald ripening may occur and lead to fluid redistribution due to progressive mass transfer over time. However the first modeling attempts indicate that multi-bubble equilibrium is possible in a porous media and that the time scales for Ostwald ripening in sandstones is on the order of magnitude of few years at least. The results from the second experiment highlight the complexity of the imbibition process. In particular, the experiment shows non-stable scCO2 over the course of the experiment with disconnected ganglia getting progressively reconnected with time. We hypothesize that fluid displacement may be caused by local capillary equilibration following the imbibition process. The detailed analysis of the temporal evolution of scCO2 ganglia also suggests that a small fraction of mobile CO2 may reconnect most surrounding disconnected ganglia.

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Pore-scale simulation of two-phase flow in porous media and upscaling: Volume of Fluid(VOF) and pore network study

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Several examples of pore-scale simulation two-phase flow in porous media are presented. Volume of Fluid(VOF) method and pore network models are employed. Capacity of pore-scale models are explored. Upscaling from pore-scale to continuum-scale are discussed.

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Surface roughness effects on calcite dissolution: Single pore models and Microfluidic Experiments

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Dissolution of calcite plays an important role in various processes such as enhanced oil and gas recovery, CO2 sequestration, and groundwater transport for the drinking water production. Dissolution rates predicted by pore scale and continuum scale models are often faster than the observed laboratory rates (Molins et.al., 2014). This discrepancy suggests that the importance of pore surface roughness. Irregular pore wall surfaces may evolve over the course of reactions, leading to changes in surface roughness and reactive surface area with time. To parameterize the irregularity of surfaces and its effect on dissolution rate, we will model single pores having different surface roughness controlled by the depth of roughness and its frequency. This roughness factor will directly be used in calculating the surface area. If the surface becomes more rough, initial reactive surface area increases. The subsequent surface area change will impact dissolution rates. Apart from the different effluent concentration of Ca2+, pores should have different solution flow velocities affecting the development of the boundary layer close to the mineral surface. This will involve coupling of solute transport with reaction kinetics in the surface layer and movement of the pore wall boundary. To develop accurate understanding of single pore processes, a number of microfluidic experiments are performed. A custom made micromodel consisting of a 2D pore network will first be injected with supersaturated CaCO3 solution. After growth of calcite at pore surface, dissolution processes will be monitored by establishing undersaturated conditions. The understanding developed from these experiments over the dissolving pore boundary will be useful in controlling model boundary velocity. The developed relations between roughness factor, surface area and dissolution will subsequently be used in pore network models using PoreFlow package (Raoof et. al., 2013). The control of surface roughness over dissolution rate at pore scale will follow the upscaling approach presented earlier (Wolthers et al. 2013) from molecular scale processes to lab sample scale calcite growth rates. Calcite surface has different structural sites (face, kink, steps) among which kink sites have maximum water interaction and this is measured through ion attachment and detachment frequencies that are rate limited by local water exchange kinetics. Kink site density is the roughness measurement at the molecular scale. These sites have different affinities for different ions in the solution depending on the space and ion size. My colleague Janou Koskamp is working on improving the effect of molecular-scale roughness on calcite growth and dissolution rates. These relations will be upscaled for a single pore and compared with the impact of pore-wall roughness observed experimentally.

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Surfactant Enhanced Mobilization of Trapped Oil in Dead-End Pores

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In the case of oil recovery, significant amount of hydrocarbons can get trapped in dead-end pores of the reservoir rock which are poorly connected to the main flow stream. Achieving the flow in these cul-de-sac structures is not possible through conventional pressure-driven mechanisms. However, concentration gradients of chemicals can be utilized as a suitable transport mechanism for these pore/fluid systems. In applications of chemical enhanced oil recovery, surfactants are used for accessing the remote zones of the porous medium by forming concentration gradients. Aqueous solutions of surfactant are injected in the porous media in order to mobilize the trapped oil phase by reducing the oil/water interfacial tension (IFT). The bulk solution of surfactant does not flow through the dead-end channels, but the surfactant molecules can diffuse into the dead-end channel, and generate a concentration gradient. As the surfactant molecules reach at the oil/water interface, the oil phase solubilizes into emulsion, and ultra-low IFTs form. Emulsification process is typically facilitated by providing mechanical energy of some form, such as slight shaking, mixing or sonication. However, in applications involving a porous medium, the miscibility is achieved within the pore space; therefore the mechanical energy may not be utilized. If the bulk liquid phases are not initially at equilibrium with each other, it is conceivable that certain dynamic processes such as diffusion, thermal fluctuations, or ultra-low interfacial tension could lead to emulsification when the phases are brought in contact without stirring. Emulsifying of all of the oil is not an effective recovery mechanism; nevertheless, some emulsification of oil into a microemulsion phase generates the desired low IFTs. Physical modelling using visual techniques can give some of the necessary descriptions leading to the proper formulation of mathematical models for the relevant recovery processes. This paper studies the mobilization of oil trapped in a dead-end pore by a surfactant solution which solubilizes the oil. Using a fluorescent microscopy technique and microfluidics allowed the investigators to view multiple phases (oil, water, and in situ forming emulsion) from a single image under fluorescent light. The emulsification rates and changes in the phase saturations were studied as a function of the chemical concentrations in the aqueous phase. It was demonstrated that the pore scale dynamics of the emulsification process are coupled to the pore scale flow regime. The surfactant used in this study has applications in chemical EOR applications; however, the findings are valid also for other engineering fields.

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The role of recirculation zones on non-Fickian transport phenomena in 3D porous media

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In groundwater engineering, remediation techniques based on the injection of nano/particles have enjoined a particular success. Pore-scale numerical simulations are a powerful tool to study transport of solutes and colloidal suspensions in porous media, and are used to derive constitutive laws tune macro-scale models.

In the Eulerian framework, the influence of the pore space geometry on transport phenomena was investigated thanks to computational fluid dynamics pore-scale simulations. Three different 3D periodic arrangements of spherical grains were used, namely face-centered-cubic (FCC), body-centered-cubic (BCC), and sphere-in-cube (SIC) packings, [1]. In Stokes regime, the transport of a conservative tracer and of particles undergoing instantaneous heterogeneous reaction were both investigated and the resulting outflow concentration (breakthrough curves) were analyzed: even if the porous media have the very same grains shape and size and the same porosity, the breakthrough curves present noteworthy differences, such as an enhanced tailing and early arrival times (Fig. 1).

The anomalous (non-Fickian) transport observed was indeed correlated with the peculiarities of the pore-space and to the presence of recirculation zones above all, [2]. The recirculation zones were detected at low Reynolds numbers and various methods, first of all a streaklines visualization (Fig. 2), were adopted to describe qualitatively and quantitatively such zones. The analysis of the angle formed by velocity and vorticity vectors proved to be particularly effective in the detection of recirculation zones, [1].

At last, simulating the transport of particles undergoing instantaneous heterogeneous reactions, the role played by the medium structure is evident also evaluating the deposition efficiency coefficient, as its behavior clearly depends on the grains packing adopted, [3-5].

After more than fifty years, the study of anomalous transport in porous media still offers a breeding ground for researches in many different fields [6]. Since in the groundwater framework the determination of this macro-scale parameter is a key factor to design effective remediation techniques, this work tries to exploit the potentiality of computational fluid dynamics to tackle the problem from the pore-scale, exploiting a practical approach.

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Using Interfacial Area and Euler Characteristic to Close Descriptions of Dynamic and Quasi-Equilibrium Two-Phase Flow

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Groundwater quality is impacted by many important engineering activities that involve dynamic processes such as groundwater remediation, enhanced oil recovery, and geologic CO2 sequestration. It is important to understand and model how these multi-phase flow processes affect groundwater quality to protect human and ecological health. Traditionally, practitioners have relied on constitutive macro-scale relationships between capillary pressure and wetting phase saturation (Pc-Sw) to define and model multi-phase flow in porous media. However, it is commonly known that these relationships exhibit hysteretic behavior and various theories have suggested the addition of another state variable to the Pc-Sw relationship to better describe multi-phase systems. The question of how flow conditions affect the Pc-Sw relationship also comes into play when describing dynamic (single-step drainage or imbibition) processes using experiments obtained under quasi-equilibrium conditions (multi-step drainage or imbibition). Thermodynamic approaches have suggested using specific interfacial area (Anw) to uniquely describe multiphase systems [1]. Some effort has been put into studying the uniqueness of the Pc-Sw-Anw relationship under dynamic and quasi-equilibrium conditions in 2D micromodels [2] and simulation [3]. Another approach is to incorporate fluid topology by means of the Euler characteristic (X) and use it to describe the history of the system [4]. We will present 3D data sets collected under dynamic and quasi-equilibrium flow experiments using dynamic x-ray microtomography at a synchrotron source. We will discuss the uniqueness of Pc-Sw-Anw and Pc-Sw-X relationships in each case and describe observations of fluid relaxation in multi-step experiments and its effect on the constitutive relationships.

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Boundary interface effects on anomalous dispersion in simulated two-phase porous media flow with upscaled correlated continuous time random walk modelling

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The development of upscaled mathematical models is essential for prediction and risk assessment in carbon capture and sequestration in saline aquifers. We adopt correlated continuous time random walks as a powerful mathematical framework that has been shown to match non-Fickian dispersion arising from intermittent flow paths in heterogenous porous media (de Anna et al. 2013).

Our focus is on a controlled comparison of non-wetting phase flow of carbon dioxide (CO2) in the presence of trapped brine, and non-wetting phase flow with a geometrically identical flow domain bounded by a solid porous matrix.

We adopt a highly efficient lattice Boltzmann method (LBM) developed by Jiang et al. (2014) for GPU-based parallel-computation of extremely large-scale multiphase fluid flow through complex porous geometries. Large porous domains compatible with periodic boundary conditions were designed to exhibit a wide, random range of pore configurations above a minimum practical LBM pore size. The wetting phase was first set to fill the entirety of the pore space. Next a drainage process is simulated where only non-wetting phase fluid enters the domain, displacing the in-situ saturated wetting phase as would an injected CO2 plume. The simulation is stopped when the average flux rate and phase saturation converge to steady-state values, meaning that capillary pressure has prevented injection of additional non-wetting phase. In this manner we generate a natural fluid phase distribution within the porous matrix. Subsequently replacing the immobile wetting phase by solid phase, before re-running the resulting periodic single-phase simulation, produces a closely related flow-scenario. Lagrangian fluid particle tracking subsequently conducted using the LBM flow fields allows analysis of the persistence and character of anomalous dispersion for the two scenarios as well as comparison of fitted correlated continuous time random models.

Despite distinct flow fields resulting from the slip versus non-slip boundary interfaces, we observe essentially identical, highly superdiffusive scaling of the second centred spatial moment. Our observation is consistent with Jimenez et al. (2015) who suggest that multiphase flows lead to highly intermittent, anomalous flow characteristics. The fact that the same dispersive behaviour is obtained for both multiphase and single-phase scenarios suggests that it results from the structural complexity of the flow paths, rather than from the multiphase nature of the flow.

Figure: Velocity fields at equilibrium flow state. Lighter colours indicate high velocity regions. The left image shows multiphase flow, while the right image shows single-phase flow where the trapped fluid wetting phase has been replaced by solid phase.

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Dispersion for non-Newtonian fluids using NMR techniques: comparison between Taylor dispersion in a tube and porous media.

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Dispersion is the mixing of a solute in a fluid flow which combines the diffusive and advective transport phenomena. Dispersion in porous media remains, today, a highly topical subject. Mixing in flow through porous media is ubiquitous in engineering research (processes, environment, oil recovery).

The nuclear magnetic resonance (NMR) provides a nearly ideal tracer method by marking and tracking the molecules in their movement. More precisely, we used the PFG-NMR (Pulsed Field Gradient NMR) technique [1] to derive the dispersion coefficients. The PFG-NMR method is now a standard method to measure the molecular diffusion coefficients. It is based on the measurement of molecular displacements between a matched pair of magnetic gradient pulses. It provides likewise a convenient means to measure dispersion coefficients which characterize the diffusive-convective transport. The average displacement of molecules regardless of the regime (asymptotic or not) is studied by the formalism of propagators (the probability distribution of displacements) (Fig.1) [2]. The cumulant method is applied to measure the average velocity of the fluid in Stokes flow regime and to determine the longitudinal dispersion coefficient.

We worked with a random pack of spherical PMMA beads (diameter =75-90µm) compacted in a plastic tube (porosity = 0.37) and we have studied a shear thinning fluid, a Xanthan gum solution at 0.2wt%. Particular emphasis is placed here on a comparison of the dispersion mechanisms between Newtonian and non-Newtonian fluids. We show that regardless the value of Péclet number (Pe = 10, 20 and 40) in a packing of beads, the dispersion is more efficient for Xanthan than for water (Fig.2). This observation was not expected given the rheology of xanthan. As a matter of fact, the opposite phenomenon is observed in a capillary tube (Poiseuille flow). The appearance of stagnant zones in the case of Xanthan (increase of the dynamic viscosity when the shear stress decreases) can explain this findings.

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Effect of grain size distribution on non-linear flow behavior in porous media

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The current study provides new experimental data on non-linear flow behavior in various uniformly graded granular material (20 samples) ranging from medium sands (d50 >0.388 mm) to gravel (d50=6.343 mm). Generally, theoretical equations relate the Forchheimer parameters a and b to the porosity, as well as the characteristic pore length, which is assumed to be the median grain size (d50) of the porous medium. However, numerical and experimental studies show that flow resistance in porous media is largely determined by the geometry of the pore structure. In this study, the effect of the grain size distribution was analyzed using subangular-subrounded sands and approximately equal compaction grades.

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Experiments, DNS, and Upscaling for Inertial Flows in Porous Media

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Nonlinear flows occur in porous media across a wide array of applications from flows in the hyporheic zone in rivers, to catalytic reactors. Although a number of empirical representations describing the relationship between pressure drop and pore velocity exists (e.g., the Forchheimer law, the Ergun equation), there has been renewed interest in this problem from perspective of the fundamental processes involved. In this work, we have adopted a program that combines experimental measurements of high-Reynolds number (Re) flows in porous media, direct numerical simulation of the flows, and theory to develop a better understanding of the nonlinear relationship between pressure drop and flow in porous media. The work presented will focus on three specific areas, as follows.

(1) Experimental Results. We will present examples of experimental measurements of the velocity field in porous media over a range of Re, ranging from inertially-dominated (but not turbulent) flows, to flows exhibiting highly chaotic turbulence within the pore space. These results were collected using index-of-refraction-matched particle imaging velocimetry.

(2) Direct Numerical Simulations. We have used an immersed boundary method to compute fully-resolved solutions to the Navier-Stokes equations in porous media up to Re approaching 1000. We will report on these results, with a particular focus on exploring how the fluid energy budget is influenced by changing Re and by the constrained geometry of the porous medium.

(3) Theory Development. Although there are currently upscaled versions of the Navier-Stokes equations in porous media (leading to nonlinear laws), these have generally only considered flows where the inertial component is important, but the flow is still laminar. We discuss some of the challenges of upscaling flows at high Re, and provide some ideas as to how upscaling can be conducted for turbulent flows.

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Macroscale modeling of gas-liquid flows within structured packings

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Columns equipped with structured packings are used in a variety of applications, such as distillation or absorption processes. The column is conceived as a highly permeable porous medium, involving a gas-liquid counter-current flow within the complex structure of corrugated sheets. Modeling transport phenomena in these systems remains an important challenge in chemical engineering science. Momentum is often modeled using variants of Darcy's law, where the effective parameters are determined via empirical or numerical analysis. Here, we investigate the modeling of momentum transport from two different perspectives.

On the one hand, we use a non-standard form of Darcy's laws with two equations, one for the gas, one for the liquid, which are coupled together to account for interfacial shear-stress at the macroscale. This is particularly relevant for counter-current flows in chemical reactors, where the gas phase can lead to the so-called flooding for high flow rates. Before flooding, which is the extreme case, shear stress is expected to contribute to the retention of the liquid phase, and to increase the gas pressure drop, impacting significantly the efficiency of the process. These coupled equations are derived from an up-scaling analysis and include additional viscous and inertial terms that are not considered in the traditional generalized Darcy's laws. We compute the solution of the problem at the macroscale using the ImPES algorithm in OpenFoam for flows in structured packings and more generally for flows within highly permeable media.

On the other hand, we use a three-equation description of mass and momentum transport, where the liquid is decomposed into two fictitious phases. This allows us to capture liquid dispersion in the column due to the dual structure of the packings, this phenomenon being key to assess correctly the liquid-gas exchange area and the efficiency of the column. At the pore scale, the two fictitious domains correspond to the two preferential paths along the corrugated sheets with exchange of mass and momentum at contact points. At the column scale, this method is in contrast with the approach that describe dispersion using a volume force capturing the radial spreading of the liquid phase. In this study, we discuss constitutive laws for the different effective coefficients and their impact on flow. In particular, we show that we can obtain a broad variety of behaviors, ranging from liquid branching to almost 1D homogeneous flows, and that our approach is suitable to predict the momentum transport in structured packings for all relevant regimes.

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Natural Fracture Characteristics of Piedemonte Field - Case Study

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Piedemonte is located in Colombia in Piedemonte License. This field has been identified as a low porosity and natural fractured reservoir with a compositional grading behavior which generates a rich gas condensate cap in the top and a volatile oil leg in the bottom in some of the compartments of the field, see Figure A.1.

This study describes the basics about the understanding and integration of geology, petrophysics and production mechanisms in the context of available information, conceptual models and correlations. This was done in order to fill the gaps where no information was available to understand and build the conceptual model of the natural fracture system of Piedemonte (PDM) fields.

Thin section images, Image and Sonic Logs, permeability from Basic Core Analysis compared with pressure transient analysis are indicators that suggest that Pauto and Floreña Fields are highly impacted in fluid flow due to the presence of natural fractures.

A new theoretical graph using a simple correlation to estimate the minimum fracture porosity and maximum spacing with different apertures was proposed and implemented. The correlation assumes a vertical well and uses the number of fractures, the dip of the fractures and the thickness of the structure to estimate the minimum fracture porosity.

It was integrated 2 small workflows in this study to 1) perform the maximum use of the capillary pressure measurements which are critical for the reservoir understanding and 2) for quality control of the transient test analysis to avoid possible misleading natural fracture interpretations.

Using the 2 workflows proposed, it was it was estimated from capillary pressure measurements that the Knudsen threshold of 0.1 suggests that the fluid flow in the tight matrix of PDM field is conventional (Darcy flow) even if the permeabilities are below 0.1 md. And interporosity coefficients in the order of 10-2 to be consistent with excess permeabilities in the order of 10 from coming from pressure transient analysis.

Also in this study, it was shown how to link information from different sources to the fracture intensity and orientation as: low tracer velocities that are highly related to the main fracture orientations and other useful correlations like excess permeability with the critical stressed fractures.

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Non-Darcian flow of shear-thinning fluids through Packed Beads and Rough-Walled Rock Fractures: prediction and experiments

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Understanding non-Darcian flow of shear-thinning fluids through unconsolidated porous media and rough-walled rock fractures is of vital importance in a number of industrial applications such as hydrogeology or petroleum engineering. Therefore, predicting the pressure drop-flow rate relationship in model porous media has been the scope of major research efforts during the last decades. Although the flow of Newtonian fluids through packs of spherical particles is well understood in most cases [1], much less is known regarding the flow of shear-thinning fluids as high molecular weight polymer aqueous solutions. In particular, the experimental data for the non-Darcian flow of shear-thinning fluids are scarce and so are the current approaches for their prediction. Different laws are available to express the deviations from linear Darcy law due to inertial pressure losses. In particular, Darcy's law is often extended through addition of quadratic and cubic terms weighted by two inertial coefficients depending on the strength of the inertia regime [2]. The relations between the effective shear viscosity of the fluid and the apparent viscosity in porous media when inertial deviations are negligible were extensively studied in the past. However, only recent numerical works [3] have investigated the superposition of both inertial and shear-thinning effects, finding that the same inertial coefficients obtained for non-Darcian Newtonian flow apply in the case of shear-thinning fluids. Given the relevance of non-Darcian shear-thinning flow, the scope of this work is to experimentally validate these results, extending their applicability to the case of rough-walled rock fractures and packs of spherical particles. An experimental study is performed to systematically evaluate for the first time the effects of fluid shear rheology on the flow rate-pressure drop relationships. The effects of polymer concentration, which determine the shear rheology of the injected fluid, have been evaluated. To do so, xanthan gum aqueous solutions with different polymer concentrations are injected through four packs of glass spheres with uniform size and two different replicas of natural fractures under Darcian and inertial flow regimes. A total of 2424 experimental data are then compared with predictions coming from different methods based on the extension of widely used Ergun's equation and Forchheimer's law to the case of shear thinning fluids, determining the accuracy of these predictions. The use of a proper definition for Reynolds number and a realistic model to represent the rheology of the injected fluids results in the porous media are shown to be key aspects to successfully predict pressure drop-flow rate relationships for the inertial shear-thinning flow in packed beads and rough-walled rock fractures. Our findings show that the experimental pressure loss-flow rate data for inertial flow of shear-thinning fluids can be successfully predicted from the empirical parameters obtained during non-Darcian Newtonian flow and Darcian shear-thinning flow in the tested porous medium.

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Non-linear transport phenomena in brain microvascular networks

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The cerebral microvascular system is key to a large variety of cerebral processes, including oxygen and nutrient delivery to brain cells as well as blood flow regulation as a function of neural activity. It plays a central role in numerous pathologies ranging from stroke to neurodegenerative diseases but the comprehension of the basic mechanisms involved is still largely incomplete. However recent anatomical and functional in-vivo imaging techniques, such as two photon microscopy together with optical manipulation of blood flow, have permitted significant breakthroughs [1]. These methods generate massive amounts of data that are difficult to interpret without proper theoretical and numerical frameworks. In this work, our goal is to develop models for hemodynamics and mass transport in the brain microcirculation, which can be later coupled with in-vivo measurement to understand and solve physiological problems involved in pathologies. To do so is challenging because the brain is a heterogeneous multiscale system with mechanisms occurring over a broad range of spatial and temporal scales. Further, mass and momentum transport are strongly coupled and exhibit non-linear behaviours, making it challenging to develop accurate macroscale models using homogenization techniques. Here, we consider the blood as a monophasic, non-Newtonian fluid whose rheology strongly depends on vessel diameter and discharge hematocrit (i.e. the volume fraction of RBCs in blood flowing through a given vessel). The repartition of RBCs between branches at bifurcations is notoriously difficult to describe, uneven and non-linear. The most popular approach consists in using empirical laws such as the one detailed in [2] to account for phase separation in simple bifurcation geometries. One important aspect of these empirical laws is that they connect flowrate and discharge hematocrit in a non-linear way, so that standard linear pore-network model may fail to capture important features of the flow and of the hemodynamics. For instance, recent work in [4] suggests that such empirical laws may yield strong non-linear effects whereby multiple stationary states with different stabilities are possible, at least for specific network configurations. In our computational framework, non-linear effects are captured using an algorithm based on an iterative solver, which was previously developed by our group (see [3]) and tested for large anatomical networks. To further assess its accuracy and the biological relevance of instabilities, we will present results of the solver for simple networks and compare these with experimental measurements recently obtained using microfluidics (illustrated in figure 1). We then go on to study larger anatomical networks that include thousands of vessels, check if instabilities can be triggered in such configurations, and evaluate their impact on the overall blood dynamics. Finally, we study oxygen transport within microvascular networks and coupling with the RBC distribution. The large size of anatomical networks makes it challenging to use numerical methods such as finite elements or finite differences directly. To circumvent this issue, we develop a mesh reduction approach. On the one hand, homogenization techniques [5] are first used to reduce the 3D transport equation inside the

vessel to a 1D axial equation with exchange terms with the surrounding tissues. On the other hand, the transport in the tissues surrounding the vessels is described via a boundary element method (BEM) inspired by Hsu et Secomb [6]. This hybrid approach allows us to significantly reduce the number of unknowns, from hundred of thousands to about a thousand for a single vessel geometry.

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Numerical and experimental determination of a generalized Darcy equation of yield stress fluids in heterogeneous porous medium

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Non-Newtonian fluids have practical applications in very different domains. Indeed, polymer mixtures, paints, slurries, colloidal suspensions, emulsions, foams or heavy oil present complex rheologies. Among the large number of different non-Newtonian fluids an important class of behaviour is represented by the yield-stress fluids, viz. fluids that require a minimum of stress to flow. Yield stress fluids are usually modeled as a Bingham fluid or by the Herschel-Bulkley equation. Yield stress fluid displacements in porous media have been subject of particular interest due to the yield-stress behaviour of heavy-oil [1] or foam [2]. Recently, it has been shown numerically [3], that in two-dimensional heterogeneous porous media the pressure-flow relation for Bingham fluids shows three different scaling regimes. Different pressure drops ΔP were applied in order to drive the fluid. The authors determined then a generalized Darcy equation by evaluating the flow in the porous structure. Three different scaling regimes were observed when plotting the flow rate as a function of the distance to the critical threshold pressure ΔP-ΔPc. For low and high pressure drops linear scaling was observed, whereas in the intermediate regime, flow rate is a quadratic function of the pressure drop. Regime I corresponds to the situation where fluid is flowing in only one channel. Here, the relation between flow rate and pressure drop is given by the non-Newtonian Poiseuille law which is linear in velocity in the case of Bingham fluids. During Regime II an increase in pressure triggers the opening of new paths and the relation between flow rate and the difference in pressure to the critical yield pressure becomes quadratic. Finally, Regime III corresponds to the situation where all the fluid has been sheared. In the present work, we simulated flow of a Herschel-Bulkley yield stress fluid in porous media of different structures by means of a Lattice-Boltzman method. We observed similar results as in [3] and showed that the existence of these three regimes strongly depends on the throat size distribution of the porous channels. Indeed, for a regular bead pack we obtained only one regime. This result for a regular bead pack has also been observed experimentally [4]. Then we investigated experimentally the nonlinear generalized Darcy equation for yield stress fluids when flowing in a natural porous medium. To this goal, Carbopol, a yield stress fluid, was injected into a Clashach sandstone of relatively high permeability. Different flow rates were applied and the pressure drop was measured. Fig. 1 shows the porous structure of a Clashach sandstone obtained by microtomography (left) and the flow rate as a function of the distance to the critical threshold pressure (right). As can be seen, three regimes can be observed experimentally for porous media with a significant throat size distribution.

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On the Understanding of the Macroscopic Inertial Effects in Porous Media: Investigation of the Microscopic Flow Structure

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Abstract Inertial flow in porous media occurs in many situations of practical relevance among which one can cite flow in column reactors, in filters or near wells for hydrocarbon recovery, etc. Inertial flow in porous media is characterized by a deviation from Darcy's law that leads to a non linear relationship between the pressure drop and the filtration velocity. In this work, this deviation, also known as the non linear -inertial- correction to Darcy's law, which is subject to controversy upon its origin and dependence on the filtration velocity, has been studied through numerical simulations.

Abstract First, the microscopic flow problem has been solved computationally for a wide range of Reynolds numbers up to the limit of steady flow (Agnaou, 2016) considering ordered and disordered porous structures as shown in Fig.1. In a second step, the macroscopic characteristics of the porous medium and flow (permeability and inertial correction tensors) that appear in the macroscale model (Whitaker, 1996) were computed. From these results, the different flow regimes were identified, namely: (1) The weak inertia regime where the inertial correction has a cubic dependence on the filtration velocity. (2) The strong inertia (Forchheimer) regime where the inertial correction depends on the square of the filtration velocity.

Abstract However, the existence and origin of those regimes, which depend also on the microstructure and flow orientation are still not well understood in terms of their physical interpretations, as many causes have been conjectured in the literature.

Abstract In the present study, we attempt to provide an in depth analysis of the flow structure to identify the origin of the deviation from Darcy's law. Unlike the previous studies reported in the literature, where the origin of inertial effects is often identified on a heuristic basis, a theoretical justification is presented in this work. Indeed, a decomposition of the convective inertial term into two components is carried out formally allowing the identification of a correlation between the flow structure and the different inertial regimes. These terms correspond to the curvature of flow streamlines weighted by the local fluid kinetic energy (see Fig.2) on the one hand and the distribution of the kinetic energy along these lines on the other hand.

Abstract In addition, the role of the recirculation zones in the occurrence and in the form of the deviation from Darcy's law has been thoroughly analyzed. For the porous structures under consideration, it is shown that: (i) The kinetic energy lost in the vortices is insignificant even at high filtration velocities. (ii) The shape of the flow streamlines induced by the recirculation zones plays an important role in the variation of the flow structure which is correlated itself to the different flow regimes.

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Polymer flow through porous media: from pore-scale phenomena to macroscopic properties

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The creeping flow of complex fluids through porous media embraces a wide variety of practical applications such as composites manufacturing [1], blood flow [2] or enhanced oil recovery [3]. Examples of such complex fluids are polymer solutions, where the large polymer molecules exhibit complex interactions with interfaces and between each others. These effects at the molecular scale may significantly affect the mesoscopic description of the fluid and the laws used for boundary conditions. For instance, non-Newtonian effects in the rheology of polymer solutions are usually observed, with purely viscous (such as shear-thinning) or viscoelastic effects. In addition to the non-Newtonian rheology, the polymer molecules are also known to “slip” on liquid/solid interfaces.

In the first part of this work, we use direct numerical simulations to study the flow of power-law with cut-off (PLCO) fluids through porous media [4,5]. In doing so, our primary goal is to better understand the coupling between the non-linear effects and the spatial length scales of the porous medium. We find that the non-linear effects only weakly impact the flow statistics and that the primary mechanism controlling the flow pattern is the geometrical constriction of the flow. We further study the transition between the Newtonian and non-Newtonian regimes and show that it can be characterized by a simple lengthscale, which is the signature of localized viscous dissipation.

In the second part of this work, we propose a theoretical upscaling of the flow of PLCO fluids with slip boundary conditions. Closure problems that are developed using this procedure are computed in a variety of media, from simple geometries to more realistic structure obtained using x-ray computed tomography. Using experimental data from coreflood tests, we find that a Navier-type boundary condition for the slip accurately describes interactions between the polymer molecules and the solid interface. We also emphasize that the permeability tensor is very sensitive to the flow direction . This is important in petroleum engineering, and more specifically in reservoir simulators, as it suggests that the traditional scaling of the permeability tensor via a scalar quantity (the effective viscosity) may fail to account for anisotropy induced by non-Newtonian effects.

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Pore scale flow fields and shear rate for sandstone rock in comparison to model geometries

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In order to improve the macroscopic sweep efficiency in oil recovery, often aqueous solutions with polymer additives are used. They typically exhibit shear thinning rheology in order to increase the viscosity in the formation but allow for a low viscosity at the injection point. In order to optimize respective polymer formulations, the Darcy-scale effective viscosity in the porous medium needs to be predicted from the bulk shear rheology. For that purpose often semi-empirical correlations such as the Cannella or Blake-Kozeny equation are used which are derived under the assumption that the porous media can be approximated by a capillary bundle for which exact analytical solutions exist. The Darcy-scale effective viscosity is then approximated by a cross sectional average of the local flow field resulting in a linear relationship between shear rate and flow velocity. The linear relationship allows to express the average/effective viscosity as a function of an average flow rate instead of an average shear rate. The local flow field, however, does in general not exhibit such a linear relationship, not even for Newtonian fluids. For capillary tubes the velocity is maximum at the center while the shear rate is maximum at the tube wall indicating that shear rate and flow velocity are rather anti-correlated. The local flow field for a sphere pack is somewhat more compatible with a linear relationship. For sandstone rocks the flow field computed from hydrodynamic flow simulations performed directly on pore-scale resolved digital images fall between the two limiting cases of capillary tubes and sphere packs and do in general not exhibit a linear relationship between shear rate and flow velocity. This indicates that some of the shortcomings of the semi-empirical correlations such as the empirical constant (“C-factor”) varying over 3 orders of magnitude and dependent on porosity, permeability, and other parameters of the porous medium originate from the approximation of the shear rate by a linear relationship with the flow velocity which is not very well compatible with flow fields from direct hydrodynamic calculations. The study also indicates that flow fields in 3D rock are not very well represented by capillary tubes.

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Slip flow modeling at pore scale and roughness in real world geometries

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When one wants to study a porous sample at microscopic scale, running simulations often requires high resolution meshes to model the whole geometry. We will expose some results aiming performing high resolution simulations, with the help of moderate computational resources.

Our studies are based on the use of hybrid methods called grid-particle methods. This kind of methods allows on the first hand to compute the velocity field on a fixed (often cartesian) grid. Velocity field is computed by solving the Stokes equation with incompressibility conditions (and constant viscosity for our study). On the other hand, the quantity of interest (for instance, a mass concentration) is carried by particles which can freely move in the whole domain. This quantity follows a transport-diffusion equation (which depends on the values of velocity) and is evaluated through a quadrature formula. This quadrature is based on a measure solution, which is a solution on a dynamical system derived from initial equation. It gives exact values at each particle in the case of pure transport.

Since the transport equation and the Stokes equation in case of inhomogeneous medium involve at the same time velocity and the transported quantity, thus we need a way to make particles and grid communicate. It is also useful to know particle data on grid points, for differential operator evaluation or for visualization purpose. The information exchange between grid and particles is performed through interpolation techniques. We retrieve the contributions with the help of an interpolation kernel by means of a convolution with the field of interest. The choice of interpolation kernels and the issues related to their use (as sign and mass conservation) will be discussed.

The particle transport and the interpolation between grids and particles are linear in complexity, hence the necessity to have an efficient 3D Stokes solver. In order to treat 3D real cases at high resolution, we will discuss how to satisfy some boundary conditions at the fluid-solid interface, like no-slip and slipping conditions to model a rough wall. We will introduce a method based on a velocity/vorticity formulation and a split of penalization and diffusion. This technique is inspired of methods used for external flows. Our contribution make it suitable for big amount of geometric data. This method splits the problem into two distinct parts: while the boundary conditions are satisfied thanks to the penalization, the diffusion part can be treated efficiently by the use of Fast Fourier Transform solver. Indeed, the FFT solver allows the number of grid points to be very large without requiring a huge memory space. When combined to coarse grid preconditioning, it shows a good convergence according to residual velocity on the fluid/solid interface inside the porous media. The cases of cylindrical Poiseuille flow, beads network and Bentheimer sample will be exposed, to illustrate the robustness of the method.

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Viscoelastic Flow Simulations in Random Porous Media

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Polymer liquids are used in the oil industry to improve the volumetric sweep efficiency and displacement efficiency of the oil from a reservoir. Surprisingly, it is not only the viscosity but also the elastic properties of the displacing fluid that determine the displacement efficiency. This may be caused by the ability of a viscoelastic fluid to pull oil out of dead-ends. The main aim of our work is to obtain a fundamental understanding of the effect of fluid elasticity, by developing an advanced computer simulation methodology for the flow of non-Newtonian fluids through porous media.

As a first step, we simulate a three dimensional (3D) unsteady viscoelastic flow through a rectangular duct of realistic pore dimension using computational fluid dynamics (CFD). The primitive variables velocity, pressure and extra stresses are used in the formulation of the model. All the mass and momentum equations are considered and discretised in space and time. The physical and rheological properties of actual polymer solutions used in polymer flooding have been incorporated, where the viscoelastic stress part is formulated using a FENE-P type of constitutive equation, which can predict both shear and elongational stress properties during flow through porous media. The simulations are performed using a finite volume methodology (FVM) with a staggered grid. The solid-fluid interfaces of the porous structure are modeled using a second ordered immersed boundary method (IBM). A coupled FVM-IBM methodology [1] is used to study flow in a three dimensional random porous medium.

The porous medium is generated by placing stationary spherical particles of equal size in random positions using a Monte Carlo method. By means of 3D periodic boundary conditions we model the flow behavior for Newtonian and viscoelastic fluids through such a porous structure. The effect of porosity and different Deborah numbers is studied in detail. The simulations provide detailed insight on how flow structure and viscoelastic stresses change with increasing Deborah (De) number. To our surprise we observe completely different flow structures at high De through various pore configurations. The simulations provide a detailed understanding of the strong interplay between fluid rheology and flow topology in a random porous medium. This work has a significant importance for applications in oil recovery, polymer and food processing, and other industries.

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Comparison Of Percolation Theory To Pore-Network Theory For Relative Permeabilities And Capillary Pressures

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Objectives: 1. Obtain realistic relative permeabilities and capillary pressures based on pore-size distribution and topology using percolation theory 2. Compare results obtained with percolation theory to results obtained with pore-network theory

METHODS PROCEDURES, PROCESS: Percolation theory seeks to describe by statistical means the morphology of, and transport through, randomly disordered media (Sahimi 1994). The theory pertains to networks that consist of branches (bonds) and nodes (sites). Here, bond percolation is considered. In this approach, porous media are approximated by a network of ducts (prisms). We use a finite-element approach to compute conductivities of arbitrarily shaped ducts, which are partly filled with oil and water. We use the effective-medium approximation to obtain the conductivity of oil and water of the whole network. We compare results obtained with percolation theory to results obtained with a pore-network model consisting of a simple-cubic lattice of prisms.

RESULTS, OBSERVATIONS, CONCLUSIONS: Percolation theory can derive realistic relative-permeability functions for combinations of different pore shapes and pore-size distributions. For water-wet systems, percolation theory shows that the intersection point of the water and oil relative permeability occurs at water saturations above 50%, as also observed experimentally. Lowering the percolation threshold shifts the intersection point to higher water saturations. Residual oil saturations increase in the sequence of isosceles triangular prisms, equilateral triangular prisms, to square prisms. Both the secondary and primary oil relative permeabilities increase in the sequence of isosceles triangular prisms, equilateral prisms, to square prisms. The water relative-permeability function shows a concave shape whereas the oil relative permeability shows a concave/convex shape. Similar to Brooks-Corey, water relative permeabilities decrease significantly as the water saturation drops below 100%, whereas oil relative permeabilities is much less affected when the oil saturation drops below 100%. Contrary to Brooks-Corey, water relative permeabilities show a marked reduction below a critical water saturation Swc, but continue to be non-zero even at very low water saturations. The capillary pressure remains finite even at low water saturations. Primary-drainage oil relative permeabilities are non-zero at low oil saturations. Comparisons indicate that network models require much larger network sizes (representative elementary volume) than conventionally used to obtain realistic relative permeabilities; in particular, near the percolation threshold.

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Computational Homogenization of seismic attenuation in fractured rock

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Fluid-saturated fractured media such as reservoir rock are well-known to exhibit pronounced attenuation of elastic waves at low seismic frequencies (f < 100 Hz), see Figure 1. The underlying process for the observed energy dissipation is the equilibration of pressure gradients in the saturated pores and fractures due to pressure diffusion between heterogeneities at the mesoscopic level (typical length scale l = 10 m). Hereby, the meso-level represents an intermediate length scale between the pore scale (micro) and the observer scale (macro), see Figure 2. These mesoscopic heterogeneities may comprise, for example, regions saturated with different pore fluids such as water, oil or gas (called patchy saturation). In other cases one observes regions in the reservoir rock with varying mechanical properties of the rock matrix (double porosity). We are particularly interested in the pressure diffusion phenomena being active in fluid-saturated fractures with extreme aspect ratios (a > 1e4 - 1e6). Since, at seismic frequencies, the wave length of the elastic waves is significantly larger than the meso-structure, the diffusion process in the saturated background rock can be described by Biot's quasi-static equations of linear consolidation. For the modeling of the diffusion processes active in the fractures having large aspect ratios, the Poiseuille flow model allows to assume a Darcy-type diffusion alongside the fractures. In this contribution we aim to introduce a computational homogenization scheme substituting the heterogeneous fractured poroelastic medium by a homogeneous poro-viscoelastic substitute model. We, therefore, establish a volume averaging concept based on the principle of macro-homogeneity [1]. Hence, the overall attenuation properties of the saturated fractured rock are computed on the basis of a mesoscopic Representative Volume Element (RVE). We solve the resulting homogenization scheme in terms of a so-called FE2 procedure. However, limited computation power as well as computational storage capacity restrict this method to artificially small computation domains. We overcome these severe limitations making use of the model's linearity and deriving a reduced order formulation for the up-scaling problem [2]. Hence, we identify a reduced basis for the pore pressure field on the small scale by a Proper Orthogonal Decomposition and superimpose the stress response due to transient external loadings. Doing so, we are able to identify a viscoelastic substitute model for the fluid-saturated rock at reasonable numerical costs. Finally, we validate the method by numerical simulations at full mesoscopic resolution.

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Continuum scale modeling of drainage process of thin hydrophilic fibrous layer

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Given the fact that thin layer is not satisfying REV length scale requirement, it is essential to better understand how to model the fluid flow process in such a medium. Recently, Qin and Hassanizadeh [1,2] introduced a new thermodynamically approach for modeling multiphase fluid in a stack of thin porous layers which is called: “Reduced continua model (RCM)”. All equations in this model are derived in terms of thickness average properties. The main objective of this study is to compare RCM to the traditional Darcy based models and improves it in order to better predict the drainage process of a hydrophilic thin porous layer. Furthermore, water dynamic in drainage process of a single thin fibrous layer has been simulated considering a dynamic term as postulated by Hassanizadeh and Gray[3].Final results of numerical simulation using RCM model show reasonable agreement compared to laboratory data . Additionally, the computational effort is decreased by one order of magnitude comparing to traditional models.

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Grain-scale investigation of REV in granular materials, using the Discrete Element Method

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In granular materials, the Representative Elementary Volume (REV) is a direct result of the particle locations, particle size distribution, and the shape of the particles. To study the REV of granular materials at the grain-scale, the Discrete Element Method (DEM) is employed to generate packings of spheres. In DEM, packings can be constructed to match a given particle size distribution and either a given porosity value or a given state-of-stress inside the packing. From these packings, hydraulic properties such as porosity, permeability and the capillary pressure – saturation curve can be computed using direct simulations, pore unit approach and/or the pore morphology method. The minimum number of particles that are required for those hydraulic properties to be independent of the number of particles can be investigated using two methods: 1) a packing is generated that contains a large number of particles, from which hydraulic properties are determined in a sub-domain that is increased incrementally; 2) a variety of packings is generated for various numbers of particles, where for each packing the hydraulic properties are computed. The latter method is convenient as typically many packings are generated for various conditions. We found that approximately 4000 spheres are sufficient for a narrow and normal distributed granular material. An additional degree of freedom arises when the shapes of particle are included, not only the particle position is important, but also its rotation and its randomness in shape. In DEM, particle shapes can be included as sets of overlapping spheres. We found that the minimum number of particles is approximately 2000 (i.e. 20.000 spheres) and that a minimum of 20 shapes should be included as otherwise the number of shapes affects hydraulic properties.

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Influence of the micro-CT images scale on the estimation of the rock properties

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In this research we analyse the effect of the micro-CT scans size and resolution on the accuracy of the macroscopic parameters estimations of the rock sample. We considered a Bentheimer outcrop sandstone sample and investigated four micro-CT scans with different resolution from 0.9 mkm to 24 mkm per voxel. The size of the images was 500x500x500 voxels, thus the physical size was strongly different. Examples of the segmented images are provided in figure. On the base of statistical analysis, we showed that if the segmented image is considered as a binary random field, statistical representative volume to estimate its properties is about 15 correlation lengths. These properties are correlation length of pore-to-matrix distribution, porosity, geometry and topology of the pore space and matrix. On the contrary, estimation of the permeability and elastic properties of rocks require much bigger samples. To overcome this difficulty, we applied truncated Gaussian field technique for statistical simulation of images. We showed that this technique allows to reproduce images with given porosity, pore-to-skeleton distribution, and permeability. However, geometrical properties of the simulated images do not match those of original CT-scans and advanced statistical simulation techniques are needed to account for the geometry of the pore space.

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Investigating Multiphase flow Behavior in Trickle Bed Reactors using eXtended Discrete Element Method (XDEM)

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The existence of multiphase flows through packed bed of solid particles in broad spectrum of engineering disciplines such as chemical industries, petroleum engineering, wastewater treatment is undeniable. One frequently used reactor of this type is a trickle bed reactor that usually contains particulate phase of which the interstitial space is filled with gas and liquid phases. Based on the direction of the fluid flow they can be classified as cocurrent downflow trickle bed reactors, counter-current trickle bed reactors and cocurrent upflow packed bubble reactors. In these kind of problems numerical simulations can help to gain a better process understanding.

In the current distribution, a numerical method so called Extended Discrete Element Method (XDEM) was applied to model multiphase flow through packed bed of solid particles which has the ability to be coupled to Computational Fluid Dynamics (CFD) through interphase momentum transfer. In this coupled solver the fluid phases are treated by CFD while the position and orientation of the particles in each CFD cell and the porosity distribution through packed bed are provided by XDEM. This capability of XDEM not only eliminates the empirical correlations but also make it possible to investigate the malddistribution pattern of liquid saturation along the bed.

In order to validate the code, two important hydrodynamic parameters such as pressure drop and liquid hold up were investigated and satisfactory agreement between predicted and experimental data was achieved. The model results demonstrate enormous effect of solid particles on the deviation of fluid phases while passing through packed beds by investigating parameters such as velocity and drag forces.

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Representative elementary volume for capillary dominated two-phase flow in porous media

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Digital rock physics, which combines high resolution imaging and high performance computation to determine the pore scale structure and petrophysical properties of rocks, has evolved significantly in the last few years and is beginning to complement and enhance traditional laboratory techniques. Its quicker turnaround time and lower cost for complicated multiphase setups, especially for multiple-scenario studies, are very attractive. The technology has penetrated not only in the petroleum industry, academia as well. High resolution X-ray micro-tomography is a major method to acquire 3D images of a rock. Due to the limitation of the field view of current x-ray micro-tomographic technique, multi-scale imaging and simulation approach has to be adopted to investigate complex heterogeneous porous media. This multi-scale approach heavily relies on whether the result of pore-scale modeling is representative and correctly identifying the representative elementary volume (REV) for the property under consideration. In our previous paper [1], we proposed a method to identify REV for capillary dominated two-phase flow in porous media by investigating the size dependences of four fluid-flow properties: trapped wetting phase (WP) saturation (Swpt) after drainage, trapped non-wetting phase (NWP) saturation (Snwpt) after imbibition, NWP saturation (Snwpbt) at NWP breakthrough during drainage, and Swanson permeability (Ks) derived from drainage capillary pressure curve. In previous investigation, we used cubic sub-samples (Lx = Ly = Lz) and did not address the effect of sample shape (Lx ≠ Ly ≠ Lz). In this presentation, we will report new results using cuboid sub-sample. The results suggest that one should use cuboid sample with longer size at the transport direction for REV of Snwpbt, which can be related to the first point of relative permeability for primary drainage (saturation value). We will also discuss the Swanson's equation and the Swanson permeability (Ks) derived from drainage capillary pressure curve obtained by digital rock physics. The agreement between the Swanson permeability and the permeability computed by Lattice–Boltzmann method would be improved if we adjust the two constants in the Swanson equation.

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Requirements for an REV identified by the concept of sufficiency using the example of capillary pressure

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Macroscopic constitutive relationships are often motivated by empirical findings or microscopic observations, e.g., capillary pressure that can be related to saturation and averaged curvature or interfacial areas. The criterion of sufficiency allows to improve such an initial constitutive relationship using only sufficient parameters as arguments. Minimal sufficiency further reduces the amount of necessary information. This concept is motivated by the Rao-Blackwell-Kolmogorov theorem in statistics and based on the conditional expectation. The concept of sufficiency can also be used to identify requirements for an REV, which is demonstrated for capillary pressure. First, the requirement and sufficiency of saturation and interfacial areas is discussed. This eliminates one-dimensional REVs as candidates, because they are able to represent volume-to-volume ratios but not surface-to-volume ratios. Second, the improvement scheme can be interpreted as an average over a larger REV or as extending a two-dimensional REV to a third dimension. The restriction to sufficient parameters further reduces the number of valid REVs and hence also reduces the effort for post processing of numerical and experimental data.

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Localized Banach Contraction Estimates for Multirate Iteratively Coupled Flow and Geomechanics Problems

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Recently, the accurate modeling of flow-structure interactions has gained more attention and importance for both petroleum and environmental engineering applications. A clear understanding of the fluid flow and the solid-phase mechanical response is needed for the accurate modeling of multiscale and multiphysics phenomena such as reservoir deformation, surface subsidence, well stability, pore collapse, hydraulic fracturing, CO2 sequestration, and hydrocarbon recovery [1]. Of particular interest is the coupling between subsurface flow and reservoir geomechanics. Different single rate and multirate iterative and explicit coupling schemes for solving the flow problem coupled with geomechanics have been proposed and analyzed in the past [2,3,4,5]. Extending the work of Mikelic and Wheeler [3], Banach fixed point contraction was established for iterative coupling schemes, while explicit coupling schemes were shown to be only conditionally stable. However, all previously established results are valid for spatially homogeneous poroelastic media. Although this is a simplified theoretical assumption, it is not true in practice. In this work, we try to bridge this gap, and consider the mathematical analysis of iterative coupling schemes for spatially and temporally heterogeneous poroelastic media. We will show that the contractivity of the single rate and multirate iterative coupling schemes extends to the localized case in which each grid element has its own set of flow and mechanics parameters. However, heterogeneities come at the expense of imposing more restricted assumptions on the number of flow finer time steps taken within one coarser mechanics time step (for the multirate iterative coupling scheme). Moreover, in contrast to previously established results, the proposed single rate and multirate iterative schemes contract on localized weighted norms, taken into account the heterogeneities of the involved parameters. Our mathematical analysis will be supplemented by numerical simulations, validating our derived theoretical assumptions.

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Scalable FS-CPR preconditioner for fully-coupled multiphase poromechanics

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The mathematical framework describing fluid flow through deformable porous media consists of balance laws for the linear momentum and mass of each phase. An implicit, tightly-coupled solution of these governing equations is frequently necessary to obtain reliable model predictions, but the development of efficient and scalable algorithms is non-trivial. Here, we describe an iterative solution framework that scales well on large computing platforms. The linearization of the system of nonlinear algebraic equations produces a Jacobian matrix characterized by a specific block structure. Based on an approximate block-factorization of this matrix, we propose a two-stage preconditioner. A generalized Constrained Pressure Residual (CPR) approach is used to construct a reduced pressure-displacement system, involving unknowns with long range error components. In the first stage, these components are addressed with a fixed-stress (FS) preconditioning algorithm and algebraic multigrid. Once pressure and displacement degrees of freedom have been updated, a second stage is applied to deal with the remaining saturation unknowns. Numerical results are presented to illustrate performance and robustness of the proposed preconditioning approach on a variety of challenging test problems.

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A digital core analysis approach for multi-rate two-phase flow using high stability lattice Boltzmann methods

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Accurate measurement of relative permeability is very important for the successful application of enhanced oil recovery techniques in hydrocarbon bearing reservoir rocks [1]. Different numerical (e.g lattice Boltzmann approach) and experimental techniques have been applied to estimate two phase petro-physical properties such as relative permeability for reservoir rock samples under different flow conditions. However, most studies on the prediction of relative permeability using the lattice Boltzmann approach have been carried out on two-dimensional samples. In this study, we consider the application of two lattice Boltzmann schemes to predict relative permeability at different saturations in realistic geometries of 3-dimensional reservoir rock samples. The advantages of the LB approach in the context of the present application are its easy implementation of solid fluid boundary conditions as well as the simplicity of its algorithm [2-4].

In our simulation, we use an imaged sample of reservoir rock for a particular fluid distribution. First, we show that our multiphase model is able to account for both fluid-fluid and fluid rock interactions. We demonstrate the model's consistency for Laplace's law formulation and its ability to predict contact angles at static conditions [5]. We then use an initialisation procedure based on a CDT morphological map for a particular saturation and threshold radius. We predict fluid behaviour for different fluid properties, namely: different density ratios and at different fluid kinematic viscosity.

The simulation model adopted for modelling two phase flow behaviour both for the imaged sample and for the morphologically based initialisation followed the single relaxation time (SRT) LB model. To increase the window of stability and check the dependence of relative permeability on the stability of the model used, we introduce the two relaxation time model (TRT) to estimate relative permeability for the 3-dimensional rock sample [6-8]. Furthermore, we consider the case of different magnitudes of body forces to drive the two fluid phases in a periodic domain. We compute the fluid interfacial tensions as well as values of relative permeabilities in both the SRT and TRT models. In addition, pressure boundary conditions are applied to drive our two-fluid system. We test the effect of boundary conditions on estimation of relative permeability. We finally carry out a test on discretisation effects by performing measurement for relative permeability at three levels of sample discretisations.

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A New Approach for Implementation of Boundary Condition in Pairwise Force Smoothed Particle Hydrodynamics

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In this work, the pairwise force smoothed particle hydrodynamics (PF-SPH) method (Tartakovsky and Panchenko, 2016) is utilized to study phenomena of multiphase flow in porous media. Unlike the multiphase SPH based on the continuum surface force model, the interfaces and contact angles are automatically captured in the PF-SPH through introducing pairwise force models.Interface construction and exerting additional force to obtain the expected contact angle are not necessary in this method. Moreover, the method is based on volumetric averaging scheme for physical variables, and problems with high density ratio and viscosity ratio are easy to deal with, which is another attractive point of this method. However, as a Lagrangian method, exerting boundary conditions in an Eulerian view becomes quite inconvenient in implementation. Periodic condition and solid boundary condition are mostly applied in previous works. In this work, to solve this problem, we propose a novel approach for implementation of advanced boundary condition, including constant inlet velocity, constant pressure for both inlet and outlet. For validation, results of several tests are compared with the traditional Eulerian methods like finite difference method for single phase flow. For applications of flow in porous media, gas-water two-phase flow is simulated based on the PF-SPH and boundary condition implementation proposed in this work, and a synthetic pore-scale matrix framework is applied. Moreover, gas-water relative permeability curves can be obtained with this method by exerting certain reasonable boundary conditions for the inlet and outlet. Finally, effects of different parameters, such as the surface tension magnitude, contact angle for the gas-water-solid system, on the two-phase relative permeability curves are also studied.

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Anisotropic breakthrough and relative permeability in fibrous gas diffusion layers: Insight from X-ray tomography and pore morphology modeling

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Understanding microstructure-property relationships of thin fibrous gas diffusion layers (GDL) is an important condition for materials optimization in PEM Fuel Cells. In this study we performed experiments with a commercial GDL (SGL 25BA) where liquid water is gradually injected from the bottom. The migration of water and associated breakthrough behavior is observed at the pore scale level by means of in-situ X-ray tomography experiments (at PSI) [1]. In through-plane direction a 'pseudo-breakthrough' is observed, whereby local bubble-points on the surface evolve continuously over an extended pressure interval. In contrast, in the in-plane direction the breakthrough is an abrupt event. The migration and breakthrough of liquid water in the fibrous materials can also be simulated using the pore morphology method. These simulations help to understand which microstructure features (e.g bottlenecks) and macroscopic properties (e.g. short transport distances through the thin layers) are critical for liquid migration, breakthrough and transport. Microstructure limitations for two phase flow under steady state conditions and associated relative permeability are also investigated with the mentioned 3D-data from in-situ tomography. For this purpose GeoDicts flow solver was used in combination with in house image analysis methods for topological characterization. Quantitative relationships have been established previously, which enable to predict permeability based on topological characteristics (effective porosity, constrictivity, geodesic tortuosity, hydraulic radius) [2–4]. For the wet GDL the predicted and simulated permeabilities are in good agreement. In contrast to literature, the relative permeability curves in our analyses show complex 'S-shapes' with concave, linear and convex segments. The shapes of these segments can be explained in the view of the mentioned continuous breakthrough behavior (at low to moderate liquid saturations) and with the detailed information from quantitative micro-macro-relationships that help to identify limiting effects from the microstructure, which are extensively discussed in two recent papers [5,6]. The findings are considered as a basis for future purposeful optimization of GDL microstructure and associated flow properties of liquid and gas phases.

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Interface-resolving CFD simulation of gas-liquid two-phase hydrodynamics in solid sponge structures

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Solid sponges are open-cell, highly porous ceramic or metal foams with a large specific surface area. These advantageous intrinsic properties promise very high heat and mass transfer rates at comparatively low pressure drops. For two-phase (gas-liquid) flows, their high specific surface area also induces an increase of the specific interface area between both phases, which is why sponges are also considered for application in separation columns or evaporators. For the design of such apparatuses, an in-depth understanding of the underlying two-phase transport processes on the pore-scale level is desirable. There have already been some experimental investigations on two-phase hydrodynamics in sponges, e.g. by means of X-ray computed tomography [1], but only few corresponding numerical investigations. This work is based on an interface-resolving phase field method which treats the gas-fluid interface as a transition layer with finite thickness. It makes use of an extra diffusive term in the phase mass conservation equation to account for the motion of the three-phase contact line on the solid surface. This numerical method has been implemented in OpenFOAM® and its reliability has been verified for simple validation cases with an analytical solution available [2]. In the following, an adequate CFD model set-up for the simulation of co-current gas-liquid flow has been developed. It is based on representative elementary volumes (REVs) of ceramic SiSiC sponges, whose geometry is reconstructed from micro computed tomography (µCT) scans of the porous structure. These REVs have been surrounded in flow direction by so-called 'thin layers' without solid structure. This special treatment eases the application of cyclic boundary conditions including a pressure fan condition to specify the two-phase pressure drop. The two-phase distribution at the cyclic patches is fixed as well, having the basic shape of a liquid jet around the REV's axis (see Fig. 1). By varying the pressure jump and the liquid hold-up at the cyclic patches, systematical variations of the flow rates of both the gas and the liquid phase may be carried out. Concerning the trends and orders of magnitude, the numerical results of this parametrical study agree well with corresponding experimental validation data [1]. Further phenomenological studies, including e.g. a variation of the contact angle on the solid surface, have been carried out to prove the reliability of the numerical method and to gain a better understanding of the underlying mass and momentum transport processes. The results and insights gained from this work form a good basis for further investigations on two-phase flow in porous media which – in a next step – shall also include two-phase heat transfer processes prevailing e.g. in flow boiling and condensation.

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Multi-GPU simulation of the impact of capillary, viscous and inertial effects on drainage displacement patterns

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To improve our understanding of pore-scale displacement phenomena and their impact on CO2 storage efficiency, we investigate the immiscible displacement (drainage) of a wetting fluid in a porous medium by a non-wetting fluid using multi-GPU lattice Boltzmann simulations, under various capillary numbers and viscosity ratios. According to Lenormand et al [1], this immiscible displacement can be characterised by just two dimensionless numbers, namely the capillary number Ca and the viscosity ratio M, which quantify the ratio of the relevant forces, i.e. the viscous and capillary forces. The wetting properties should also be considered via the equilibrium contact angle. With regards to inertial effects, although the average fluid flow is at low Reynolds numbers, these might be also be important over a transient amount of time, for example during Haines jump events [2,3,4]. Therefore, it would be reasonable to question whether the above description in terms of the capillary number and the viscosity ratio, could be sufficient to describe the two phase flow behaviour. If not, then we must investigate to what extent dynamical effects like Haines jumps can affect the fluid flow and, in the context of CO2 geological sequestration, affect the CO2 saturation.

Here, we demonstrate that the description based on the phase diagram of Lenormand et al [1] is not sufficient, especially in situations where dynamical effects, like Haines jump events [2,3,4], can affect the two-phase fluid flow. We propose that another dimensionless number, the Ohnesorge number, is required to fully describe the fluid flow. The Ohnesorge number describes the ratio of viscous forces over inertial and capillary forces. In numerical modelling, as there is more freedom in choosing simulation parameters compared to the experiments, tuning these parameters appropriately and matching the relevant dimensionless numbers is essential in order to correctly resolve the fluid flow dynamics. We then verify the existence of the three typical fluid displacement patterns, including viscous fingering, capillary fingering and stable displacement. We examine how these distinctively different flow regimes can affect the saturation of the non-wetting fluid when this reaches the outlet of the simulation domain.

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Multidimensional exact solutions for two-phase flow in porous media

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In general, analytical solutions serve a useful purpose to obtain better insights and to verify numerical codes. For flow of two incompressible and immiscible phases in homogeneous porous media without gravity, one such method that neglects capillary pressure in the solution was first developed by Buckley and Leverett (1942). Subsequently, McWhorter and Sunada (1990) derived an exact solution for the one and two dimensional cases that factored in capillary effects. This solution used a similarity transform that allowed to reduce the governing equations into a single ordinary differential equation (ODE) that can be further integrated into an equivalent integral equation. We present a revision to McWhorter and Sunada solution by extending the self-similar solution into a general multidimensional space. Inspired by the derivation proposed by McWhorter and Sunada (1990), we integrate the resulting ODE in the third and higher dimensions into a new integral equation that can be subsequently solved iteratively by means of numerical integration [1]. We developed implementations of the iterative schemes for one- and higher dimensional cases that can be accessed online on the authors' website [3.4]. Additionally, we demonstrate the ability of the semi-analytical solution to be used in the numerical analysis of numerical solutions in 1D, 2D, and 3D, and discuss practical difficulties associated with their use [3].

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New analytical expressions for relative permeability curves of immiscible two phase flow in a rough fracture

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Relative permeability curves for two phase fracture flow has been a subject of study in recent years. This topic is important in multi disciplines, e.g. water subsurface resources, geothermal energy, underground hydrocarbon resources especially fractured oil and gas reservoirs, and hydraulic fracturing. There are many experimental as well as numerical studies on this subject in the literature. However, simple analytical and practical solutions are still attractive. In this study, it is tried to apply wettability effects and phase interference explicitly in a simple analytical formula. The wettability effects are represented with residual saturations that resulted in direct calculation of relative permeability end point of the non-wetting phase. In addition, the phase interference part affects the curvature that enables us to quantify the degree of phase interference from no phase interference, assigned as zero, to ultimate phase interference, assigned as infinity. In addition, this parameter could form relative permeability curves which have curvature in some saturations and are linear in other parts which is observed quite a bit in experimental studies. Furthermore, the results were compared with the experimental data available in the literature to validate the method. Moreover, the formulation proposed here is applicable to both smooth and rough fracture assemblies.

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Pore Morphology Method with Hysteresis Effect for Enhance Oil Recovery Applications

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Two-phase properties of natural rocks depend on the physical history of the reservoir. Oil that invades a fully water saturated rock (primary drainage) leaves a residual water saturation. If water invades the rock again (imbibition) then residual water may reconnect to the invading water phase. Repeating both processes (secondary drainage …) yield a hysteresis. This hysteresis has minor or no effect in highly porous materials but it has a major effect in low porosity rocks. It is significant for capillary pressure curves and other relative properties (e.g. relative permeability). Therefore, this should be considered in Enhanced Oil Recovery applications.

The pore morphology method, also known as method of maximal inscribed spheres, allows predicting the distribution of a wetting phase (here: water) and a non-wetting phase (here: oil) inside a porous medium. The method distributes the phases by using morphological operations rather than solving partial differential equations. Therefore, the method is very fast and the memory requirements are very low. For drainage, spheres that represent the oil phase are placed inside the pore space where the pore size is greater than a certain radius and the pore space with this property is connected to the supply of oil on the domain boundary. The radius is decreased in an iterative process while the capillary pressure is increased. The remaining pore space describes the distribution of the water phase. The output of the algorithm is a finite sequence of quasi-stationary states. Each state is a 3D image that encodes the water and oil distribution inside the porous rock. Finally, the Young-Laplace equation based on the radii of the inscribed spheres and the interfacial tension is used to predict the capillary pressure curve. Connectivity checks with respect to the oil reservoir ensure that the invading oil phase must be connected to the oil reservoir. While connectivity checks with respect to the water reservoir allow the algorithm to introduce residual water phases where parts of the water phase are trapped and cannot leave the domain. Thus, it is possible to simulate a primary drainage process where oil drains water with a residual water phase. But the original pore morphology method is not able to capture this residual water phases as an input to a following imbibition simulation where water invades the structure and may reconnect to the residual water phase.

In this presentation, we will present an approach how to extend the pore morphology method with additional connectivity checks such that initial residual phases and thus hysteresis effects can be considered. This enables us to simulate primary drainage, imbibition, and secondary drainage experiments. We show how these hysteresis effects influence the capillary pressure and relative permeability curve.

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The chaotic gas-liquid two-phase flow in single fracture and its mechanism

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The transport of gas-liquid two-phase flow in single fracture is a very common phenomenon in nature. In this paper, many physical and numerical simulation results are presented. Chaos is found in this transport at a given situation, its mechanism is explained and the critical condition of the chaos is presented. A stochastic gas-liquid two-phase mixing flow seepage model and its numerical simulation in single fracture are presented and a horizontal Hele-shaw experiment was carried out. The numerical simulation and experiment results show that the transport chaos of gas-liquid two-phase flow happens when the relative saturation is in the range of gas relative saturation 44%-70% and its occurrence probability can be expressed in polynomial. The chaos probability exceeds 80% when the relative saturation of gas is 40%-65% and the chaos probability is 100% when the relative gas saturation is 57%-60%. The mechanism of chaos transport is: the stochastic variation of gas connection cluster and the compressibility of gas make the pressure gradient of the gas-liquid flow change both in magnitude and direction violently, then the turbulent flow is formed, the kinetic energy decreases gradually and the flow is stopped at last.

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WET GRANULAR FLOW CONTROL IN A ROTATING DRUM

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The presence of liquids has a significant effect on the dynamics of granular flow. Using a combination of experimental study and discrete particle method simulations (DEM), we investigate the effect of capillary force, liquid viscosity and particle size on wet granular flows and we establish a methodology that ensures the control of the bed flow motion in a rotating drum.

The velocity profile of the particles in the rotating drum is determined using particle tracking method and compared to the DEM simulation results. Capillary and viscous forces are included in the DEM model to describe the interactions between surface-wetted particles.

We show that the strength of capillary force between two adjacent particles can be altered through surface modification of the glass beads, thus, under the right conditions; we demonstrate that the bed flow motion can be controlled. Liquid viscosity effect on the bed flow motion is also investigated under low capillary forces. The capillary force between the particles is significantly reduced by making the glass beads hydrophobic via silanization.

The simulation and experiment results were comparable in terms of the flow patterns and dynamic angle of repose. We find that liquid-induced cohesion increases the width of the flowing layer and the dynamic angle of repose. However, it decreases the particle flow velocity in the drum. We were able to obtain similar bed flow motion for different particle sizes and the flow control methodology is found to be robust in the studied flowing regimes.

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An adaptive pore network model to characterize the flow regime domains for several rocks

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Pore scale simulation is more and more used to study various pore scale phenomena that cannot be reproduced by conventional Darcy-based simulators. Direct numerical simulation of Navier-Stokes equations on systems larger than few millimetres is impractical due to the time it would require. As a result, pore network models are a way to study the flow at the pore scale for a Representative Elementary Volume (REV). Pore network models can be divided into dynamic and quasi-static models. Whilst dynamic models explicitly consider the competition between capillary and viscous forces, they can be computationally expensive as they require computing the pressure gradients. At low flow rates, the displacement tends to become dominated by capillary forces meaning that simple flow rules can be defined to determine the filling order and the pressure calculations can be avoided. Whilst they are very efficient computationally, the usage of these models is limited to capillary dominated flow regimes obtained generally at low capillary numbers.

We propose to combine the two approaches in an adaptive algorithm taking advantage of the speed of quasi-static algorithms when the flow is governed by the capillary forces and that can simulate the viscous effects when they are important. We propose an automatic criterion to localize the pressure solution to the important areas in order to enhance the computational efficiency of the algorithm even in viscous dominated regimes.

In this paper, we first describe the adaptive algorithm used in this work. Then, we present several test cases where we show that the algorithm can improve the computational performance of the pore network simulator without losing accuracy of the solution. This algorithm is subsequently used to draw regime diagrams for several rocks at several wettability scenarios (oil-wet, water-wet and mixed-wet) where the boundaries of each flow regime are determined using an automatic criterion and plotted as a function of the capillary number and the viscosity ratio. These diagrams are particularly useful to provide a fast characterisation of the flow regime for the considered rocks under particular flow conditions and rock/fluids properties.

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Drying of a thin hydrophobic porous medium bounded with a gas purge channel

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Drying in porous media is of interest to many research and engineering fields, such as recovery of volatile hydrocarbons from underground oil reservoirs, remediation of contaminant soils by vapor extraction, and water management in gas diffusion layers (GDLs) of proton exchange membrane fuel cells (PEMFCs). In PEMFCs, produced water may condense and fill open pores of a cathode GDL, which impedes the transport of reactant gas to the reaction sites and hence is adverse to the fuel cell performance. In particular, at low temperature environment, liquid in the GDL can freeze to form ice crystals, which will damage the GDL structure and deteriorate the performance and durability of PEMFCs. To this end, it is necessary to remove residual liquid in the GDL after the shutdown of PEMFCs. A common method is to purge the dry gas into the gas channel (GC) of a PEMFC to remove liquid in the GDL through the evaporation mechanism. However, the gas purge is parasitic and consequently reduces the efficiency of PEMFCs. To reduce parasitic losses and increase the system efficiency, it is important to understand the detailed evaporative liquid removal from GDL during the gas purge. In PEMFCs, the cathode GDLs are thin (~250 μm) and treated with hydrophobic agent PTFE. In this regard, GDL drying can be taken as drying of a thin hydrophobic porous material bounded with a gas purge channel.This type of drying also can be found in other fields. To investigate this type of drying processes, a pore network model is employed. The GDL is conceptualized as a pore network (PN) composed of cubic pore bodies connected by cylindrical pore throats. Initially, the PN is fully saturated with liquid water. Then dry gas is flowed into the GC, during which liquid in the PN is removed by evaporation. The gas flow in the GC is considered as a fully developed laminar flow. The vapor transport in the channel is described by the convection-diffusion equation. The vapor transport in the PN is dominated by the diffusion. Both viscous and capillary effects are considered for liquid flow in the PN. The “capillary valve” effect is also taken into account to illustrate the movements of gas-liquid menisci in the pores of PN. Fig. 1 shows variation of liquid distribution in the PN during drying. The Reynolds number for gas flow in the GC is 100. Liquid in the PN is shown in red, and the GC is sketched by the green lines.

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Investigating Transport Phenomena in Polymer Electrolyte Membrane Fuel Cell Bilayered Gas Diffusion Layers Using Pore Network Modeling

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The polymer electrolyte membrane (PEM) fuel cell is a promising energy conversion device, suitable for a wide range of applications, including fuel cell electric vehicles and stationary backup power. The gas diffusion layer (GDL) facilitates the transport of heat, electrons, reactant gases, and liquid water in the PEM fuel cell. The GDL is a highly porous material composed of arrays of carbon fibers, coated with polytetrafluoroethylene (PTFE) to render the material hydrophobicity (1). The carbon substrate is typically coated with a micro-porous layer (MPL), which is used to reduce contact resistance between catalyst layer and GDL, as well as optimizing water management (2).

The oxygen diffusivity of the GDL is a unique characteristic of the material, evaluating the oxygen diffusion through GDL to the reaction cites. Numerical techniques have been high valuable for investigating the oxygen transport through the porous medium (3, 4). Pore network modeling is a pore-scale numerical approach of simulating multiphase transport whereby complex pore spaces are represented by a simplified network of pores connected with throats (5). Equivalent pore networks extracted from micro-CT images can be used to predict the oxygen diffusivity in the carbon substrate of GDL. However, due to the length scale disparity between micro pores within the carbon substrate and nano pores within the MPL, simulating transport phenomena in bilayered gas diffusion layers may lead to a significant computational burden.

In this work, a hybrid pore network model for investigating oxygen diffusion of bilayered GDL materials was presented. A voxel-based network of continuum MPL elements and discrete pores in the carbon substrate is created for pore network modeling, as present in Figure 1. The oxygen diffusion results were validated by comparing our pore network modeling results to the analytical solution. The preferred MPL element size for obtaining accurate results with minimal computational burden is suggested. The result of this work provides an architecture for incorporating realistic MPL structures into the pore network modeling frame, enabling the in-depth simulation of oxygen and water transport in bilayered GDLs.

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Modelling capillary dominated two-phase flow through porous media using a multi-stage generalised network modelling workflow

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Predicting two-phase flow through porous media is a challenging task. The flow regime depends on fluid and rock properties such as viscosities and density ratios, wettability and flow rates. More importantly, the flow domain has heterogeneities at various scales ranging from roughness and chemical heterogeneities on the walls of pore space and variations in the pore-size and shape at sub-micron scales to field-scale variations in the rock properties. Due to the uncertainty in these model parameters, a deterministic description of flow is inadequate and an efficient modelling tool that can be used to quantify the effect of these uncertainties is needed. We will present a multi-stage generalised network model work-flow which aims to accurately model two-phase flow covering nano-scale pores up to core-plug scale heterogeneity. We validate our model using direct simulations and fluid distributions obtained using micro-CT imaging of two-phase flow experiments at the pore scale as well as using experimental measurements of relative permeability and capillary pressure curves, while taking into account uncertainties in the input model parameters. We illustrate how this method can be used to efficiently and reliably quantify the effect of pore-scale parameters on large-scale behaviour of two-phase flow through porous media.

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Multiscale Pore Network Method for Unstructured Networks

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Dynamic pore-network models are important in studying several non-equilibrium multiphase-phase flows in porous media, such as two-phase flow at high capillary numbers and chemical dissolution of porous media by reactive fluids. However, dynamic pore-network simulations are significantly more expensive (computationally) than quasi-static pore-network simulations. The reason for this is two-fold. First, a linear system of equations is required to be solved for the pressure equation at every computational time-step. Second, the time-step criterion becomes restrictive as the pore-network size increases. In order to overcome these restrictions, the multi-scale pore-network (Minisymposium PN) method was developed. The Minisymposium PN method consists of three main steps. First, an approximate solution to the pressure problem using the multiscale finite volume (Minisymposium FV) method is computed. The computed node pressure values lead to conservative fluxes across pre-defined sub-network boundaries. Second, these conservative fluxes are used as boundary conditions to solve local problems on the sub-networks. Third, once these local problems are solved, the coefficients in the pressure problem can be updated. The Minisymposium PN method is capable of simulating flows in unstructured pore-networks with arbitrary coordination number distribution. Furthermore, since it is amenable to parallel processing, the Minisymposium PN method is potentially capable of simulating flows in pore-network domains of sizes comparable to that of core samples used in laboratory experiments. This is important in extracting meaningful macroscopic quantities, as the effects of micro-scale heterogeneity may not be apparent in smaller domains.

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Multiscale pore network modelling of imbibition: scanning curves and wettability change modelling

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The determination of static and dynamic properties in complex rocks, such as carbonates and clay rich sandstones, is strongly affected by heterogeneities at different scales. Complex depositional and diagenetic processes have a strong control on the pore structure, leading to systems with a very wide range of pore sizes covering many orders of magnitude in length scales, which cannot be captured by a single resolution micro-CT image. In the present work we present a multiscale imaging and modeling workflow to compute transport properties of rocks with a broad pore size distribution. A dry/wet micro-CT imaging sequence is used to spatially map the porosity and connectivity of macro- and micro-porous regions. The 3D porosity map is transformed into a multiscale pore network model where macro pores (resolved) are modeled in a conventional pore network manner while micro-porous network elements are treated as a continuous porous medium. In addition, high resolution BSE images are used to construct representative 3D micro-porous models, in which normal pore-network simulations are performed. These models describe the different micro-porosity regions through a set petrophysical properties (porosity, permeability and cementation exponent) and saturation dependent curves (Leverett J-function, wetting- and nonwetting-phase relative permeabilities and resistivity index). Only one set of saturation curves is used during primary drainage. However, during imbibition, as every pore has a different saturation state, a different set of saturation dependent curves needs to be used for each pore in order to properly characterize the imbibition process. A new methodology to handle this effect is introduced. In addition, several wettability change scenarios at the different scales are proposed to represent water-, mixed- and oil-wet systems. Several numerical test cases are used in order to validate this new methodology. Finally, the new multiscale workflow is applied to different heterogeneous rock samples. Simulated fluid distributions during drainage and imbibition are compared directly with those observed in micro-CT images acquired during miniature core-flooding experiments. Computed petrophysical properties as well as capillary pressure and relative permeability relationships are compared with high quality available experimental data. The agreement between computed and measured results is encouraging.

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Network modelling of immiscible two-phase flow in porous media

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We present an updated version of a dynamic pore-network model based on the original models of Aker et al. [1] with later extensions by Knudsen et al. [2]. These papers describing the model at that stage in detail were published more than 15 years ago and the model has changed significantly since then. An updated detailed paper is due. A review article on pore-scale network models was recently published by Joekar-Niasar and Hassanizadeh [3] giving an overview of available network models, the original model included.

We address some of the original model's shortcomings and we present solutions fixing these. Our updated model primarily focuses its attention on the redistribution of fluids when menisci reach an intersection of tubes in the network in such a way that it can reproduce dynamic phenomena such as ganglion dynamics [4] in a consistent manner.

We also address the extension of the model to capture the flow of films in corners, as done initially by Tørå et al. [5] for the original model.

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Pore network simulation of water condensation. Application to gas diffusion layer of PEMFC

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The understanding of water transport in PEMFCs is still a major challenge in direct relation with durability and water management issues. We concentrate on the water transfer mechanisms occurring in the gas diffusion layer (GDL) on the cathode side. The work is based on the key idea that water condensation plays a major role in the liquid water formation in the GDL. Condensation in the GDL is studied numerically from three dimensional pore network simulations at the rib - channel scale. The physics is as follows. Water produced within the catalyst layer enters the GDL in vapor phase, is transported by diffusion in gas phase within the GDL until reaching the bipolar plate channels. Next to the channels, the rib collects heat and electricity from the GDL. Under typical operating conditions, the area under the rib is the colder region of the GDL and thus a preferential place for condensation. In agreement with experimental observations, our model first shows that all the water produced can be transported without occurrence of condensation, i.e. through a dry GDL, for sufficiently low current densities and relative humidities in the channel. Liquid formation by condensation occurs when the current density and/or the channel relative humidity are sufficiently high. The conditions leading to condensation are summarized thanks to the concept of condensation diagram. When the conditions for condensation to occur are met, our model simulates the growth of condensed water clusters, taking into account the mechanisms of capillary coalescence between the water clusters, until liquid clusters reach a steady state where condensation is exactly balanced by evaporation at the boundary of each cluster. Our model leads to results in agreement with several experimental in situ observations.

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Pore-network modeling within the framework of DuMux and DUNE: A flexible, fully implicit approach with the possibility of coupling to other models

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Pore network modeling can be used in various applications to investigate flow and transport processes on the pore scale. We present a fully implicit pore network model which is included into the numerical simulator DuMux (Flemisch et al., 2011; Hommel et al., 2016). Like standard DuMux models, the pore network model can deal with various flow and transport schemes including two-phase, multi-component flow and energy transport in the fluid phases. This allows to efficiently use great parts of the numerical infrastructure readily available, like a description for wide range of fluids and components, different kinds of linear solvers and a heuristic time stepping scheme. We rely on dune-foamgrid (Sander et al., 2015), a grid interface implementation for one- and two-dimensional grids in a physical space of arbitrary dimension.

Being within the framework of DuMux, the pore-network model can be coupled with comparatively low effort to existing REV based and free-flow models which opens a broad range of potential applications such as soil evaporation, fuel cell water management and root water uptake within an agricultural context. With these multi-scale capabilities, our model can be an interesting option for modeling unconventional porous materials where processes must be regarded and treated explicit on different scales (Scheibe et al., 2015).

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Pore-scale modeling and upscaling of transport in hierarchical porous materials

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Modeling transport phenomena within unconventional porous media is of particular interest because of its vast and diverse applications such as in supercapacitors, tissue scaffolds, fuel cells, and etc. In many cases, the porous domain is microscopic, heterogeneous and/or hierarchical, meaning that single values for effective parameters like porosity or effective diffusivity cannot be obtained. In these cases, classic continuum volume-averaged approaches are not suitable for modeling reactive transport. In this work, a general framework based on pore networks for modeling reaction-diffusion in porous materials with hierarchy of porosity is presented. The pore network approach maps the porous domain into a network of void spaces (pores) that are connected through virtual tubular bodies (throats). The main advantage of pore network modeling is that effective parameters are no longer needed since transport equations are solved at pore resolution. The model is demonstrated in the context of a nanoporous particle interlaced with macropores that result from the use of porogens. Simulations show that the structural features of the porous material (ex. macroporosity) significantly influences its bulk properties such as net reaction rate. Specifically, as the macroporosity increases, depending on the local Damköhler number, the net reaction rate shows three distinct trends: monotonic decrease, monotonic increase, and mixed behavior. Finally, an upscaling strategy is proposed and implemented to extend the pore-scale simulation results to larger length scales.

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3D - Reconstruction of Porous Media using Generative Adversarial Neural Networks

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Modern computer tomographic methods enable the observation of multi-phase flow behavior of fluids in porous media. At the pore-scale, that is the scale at which individual pores in a porous medium can be resolved), many factors governing the multi-phase flow behavior occur due to interaction of the in-situ fluids with the surrounding solid structure. While Micro-CT imaging acquires “voxellized” 3D-representations of the pore-solid structure, evaluation of the associated variability of the obtained measurements at various scales must be quantified through the generation of 3D representative samples of the porous media . We present a novel method to reconstruct the solid-void structure of porous media by applying an unsupervised generative neural network that allows an implicit description of the conditional probability distribution presented by the three dimensional micro-CT image datasets. We show, by using an adversarial learning approach for neural networks, that this method of unsupervised learning is able to reproduce physically representative samples of porous media and their statistics. We successfully compare pore morphology, two-point statistics and directional single phase permeability of synthetic realizations with the evaluated properties of the acquired Micro-CT images. Our results show that generative adversarial neural networks can be used to reconstruct high resolution 3D images of porous media at different scales that are representative of the morphology of the 3D Micro-CT images. The fully convolutional nature of the trained neural networks allows the generation of large samples while maintaining computational efficiency. Compared to classical stochastic methods of image reconstruction, the implicit representation of the learned data distribution, can be stored and reused to efficiently evaluate the ensemble physical properties of 3D porous media.

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Combine multi-scale digital rock images and upscale properties using machine learning

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Machine learning has recently accelerated advances in many industries. Examples include autonomous car technology, automatic localization tumor/cancer in medical imaging and image recognition in search engine to name just a few. Oil and gas exploration industry can easily benefit from advances in machine learning, especially deep learning. Digital rock physics (DRP) provides understanding of reservoir rock properties. The process starts by digitalizing rock samples using desired resolution and field of view. Due to limitations in imaging technology and multi-scale nature of rocks, in the past less than 1% of a rock sample area will be digitalized and characterized. Undoubtedly, relevancy and representativeness of DRP are hotly debated topics for years. An approach able to characterize representatively large rock sample while requiring economic resources in term of accuracy, time and cost is highly desirable. This paper presents an approach that combines advances in DRP and machine learning for achieving understanding of rock samples at a practical scale - not only a part of it at a tiny scale. The approach is based on an understanding that a rock consists of multi-scale textures (i.e. rock fabrics, building blocks) intermixed spatially. A texture that is larger than the resolution being used will be resolved while a texture smaller than the image resolution will be unresolved. Nevertheless, unresolved image pixels/voxels still contain information about the textures. Knowledge of each of these textures together up to the sample scale leads to understanding of the whole rock. We developed an unsupervised machine learning algorithm that can identify number and location of existing textures in a rock sample. It automatically suggests areas for higher resolution acquisition of two- and/or three-dimensional images. Consequently, a trained deep learning algorithm is used to segment the high resolution images. Then DRP analysis is used to study properties, such as porosity, pore size distribution and transport properties, of the high-resolution images. Combining the DRP analysis with rock texture knowledge, rock properties can be accurately upscaled. In a case that the rock textures are not resolved by the high-resolution images, the process can be repeated recursively to study the rock at smaller scales. We demonstrate the application of the developed approach with complex rock samples. Rock textures as recognized by our machine learning algorithm will be presented as well as verification of the upscaled properties (porosity among other properties). Additionally, the approach is semi-automated requiring only minimal resources.

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Critical size of REV and resolution of digital rocks for unconventional resources

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CT scan techniques are widely used to obtain rock structures in oil field. Rock properties can then be acquired numerically. In theory and practice, REV is important in the fact that properties at this size can be representative[1]. For conventional sandstones, REV can be determined from small size and low-resolution CT images due to its relatively large pores and good connectivity[2, 3]. However, when it comes to unconventional sandstones, the image resolution has to be high enough to capture the small pores, which will decrease the physical size of the rock sample and the sample risks losing representativeness[4]. Taking into account that small pores play relatively little role in percolation process, a critical resolution may exist below which the pores can be ignored and REV isn't affected much. In this study, CT images of tight sandstone at resolution of 0.28μm are analyzed to find the REV size of porosity, tortuosity and permeability. By resampling the images, the resolution effect on REV size and properties is investigated and a critical resolution is found. The result shows that REV size can be determined from CT images but the image size has to be larger than 8003. When image resolution changes, REV size and properties also change but within 50% range, which shows that REV can actually be obtained with images larger than 2003 at resolution of 1.12 μm. This implies that a critical resolution may exist when determining the REV of digital rock for unconventional resources.

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Digital Rock Physics: Elastic property upscaling using a combination of multi-resolution Micro-CT imaging and refined moduli input through Nanoindentation

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Digital Rock Physics (DRP) is an emerging technology that consists of three major components: 1) imaging of the rock sample using high resolution 3D scanning techniques (e.g. micro CT, FIB/SEM), 2) Digitization of the images by segmenting the pore and matrix phases 3) simulation of the desired physical properties of the rocks such as elastic moduli and velocities of wave propagation.

Despite the advancement in imaging resolution yielding fairly detailed microgeometry, and the progress in numerical algorithms, studies reporting full technical details of elastic simulation are rare and accurate predictions are only seen in studies working with very homogeneous sandstones. The discrepancy is particularly higher in carbonates which have complex pore structures at multiple length scales from tens of nanometers to several centimeters. We use a multi-resolution (1 µm to 40 µm) Micro-CT imaging protocol to capture pore ranges across the different scales of a real reservoir carbonate rock. Using a FEM [1] method that assumes linear elastic and isotropic medium, numerical simulation upscaling of the elastic properties is performed. The bulk and shear moduli of the different phase materials are required inputs for the simulation. For greater accuracy of the poro-elastic simulations, information about the unresolved phase (containing nano pores below 1micron that cannot be visualized using Micro-CT) is important [2]. Currently we bulk them under grain or pore phase as their elastic properties are unknown. As a first approach to bridge this gap, in this work we will be integrating experimentally measured local elastic modulus through a technique called instrumented nano-indentation [3]. A Berkovich tip type is used to make indentation mapping over the region of interest. Through continuous depth and load sensing analysis the elastic moduli at the indentation points are determined. These results are used to enhance the predictions of the upscaled elastic simulations. Simulation results are compared against experimental elastic modulus through acoustic velocity measurements on the same rock sample.

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Digital Rock Physics: Using Artificial Neural Network to Classify Permeability Values Based on Inherent Rock Properties

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With Digital Rock Physics (DRP) complementing lab experiments in the oil and gas industry, it's proving to be a powerful tool to understand how microstructural properties affect macroscopic properties[1,2,3]. There are various challenges that still exist in DRP due to imaging and computational limitations. In the former, a high-resolution image can only be achieved for a relatively small field of view. In the latter, computational capabilities are still inefficient when it comes to determining properties at the complete standard core plug size for which experimental results exist. These challenges are exacerbated when carbonate rocks are studied due to the heterogeneity that exist at various scales. In this work, a carbonate rock sample is divided into multiple smaller cubes that undergo the basic DRP workflow of imaging, segmentation, characterization of the microstructure and computation of permeability using the Lattice Boltzmann Method. Then one-fourth of the cubes are used to train an artificial neural network (ANN) to classify them using inherent rock properties such as porosity and specific surface area as input and using permeability categories as output – three categories are defined for low, midrange and high permeability. Then three-fourths of the cubes are classified using the ANN. Finally, a Darcy-flow simulator is used to rebuild the complete rock dataset and determine its final permeability using two methods: exact permeability values for each cube and classified permeability values determined by the neural network. Results show that property values computed for both methods are comparable.

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Multi-scale imaging of shales: Impact of sand on permeability and porosity

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The evaluation procedure whether clay rocks can be used as host rocks for repositories of nuclear waste or as reservoir rocks commonly involves transport modeling to predict the sealing behavior/reservoir quality of porous sedimentary rocks up to the repository/reservoir scale. During recent years several tomographic imaging methods, which cover a wide range of scales from the nanometer to the millimeter/centimeter, were applied to samples from the Opalinus Clay unit. The paramount goal of using tomographic methods at different length scales is to establish a hierarchy of models that allows upscaling rockphysical properties. This work presents an approach for upscaling permeability from the pore scale to the overlying scale, where pores cannot be resolved and the geometry of the porous clay matrix considered as a whole controls transport properties. Microstructures reconstructed from multi-scale image data are cellular models with different sizes of basic building blocks, the so-called voxel. Flow simulations were performed on the base of the grid that is naturally inherent in the coarse scale image data that was acquired by synchrotron X-ray computed tomography. The coarse scale spatial distribution of permeability was determined on the base of local permeability distributions, which in turn, were determined on the base of the fine scale image data (the pore scale) that was acquired by Focused Ion Beam nanotomography. Then, coarse scale microstructures with different clay matrix contents were used as input for flow simulations, which allowed predicting the vertical and horizontal permeability at the mesoscale as a function of the clay matrix content. It turned out that vertical permeability kv decreases with increasing clay content, which can be explained in that the presence of coarse non-clayey grains increases vertical pore connectivity when compared to fine-grained shales. Horizontal permeability kh is generally higher than vertical permeability and increase with increasing clay content. Mesoscale permeability anisotropy kv/kh decrease from about 0.5 to 1e-3 if the clay content increases from 0.2 to 0.8. The predicted permeability behavior is discussed and compared to results from experiments and other predictive models.

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Scale Coupled Upscaling of Multiphase Flow in Digital Core Analysis

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In digital core analysis different imaging technologies are employed to identify pore or textural structures scaled from millimeters to nanometers. In each resolution the field of view of 3D image volume is up to a few thousand pixel sizes in each dimension. Utilizing a highly efficient pore scale simulator and a powerful computer cluster, the 3D rock volume that can be practically handled in a multiphase flow simulation is about one thousand pixel sizes in each dimension. It is a big challenge to compute the multiphase flow properties in these digitized rocks. A common approach is to compute multiphase flows in different regions and different scales independently and then upscale in a separate operation to get the multiphase flow properties of the whole rock sample. There are two drawbacks in the common approach. The dynamic flow exchanges in different scales are ignored. Especially the flow path and the wettability changes provided by the region of finer scale that are important for coarser scale computations are ignored. Another drawback is that the overlap pores in images of two neighbor scales in the same region are not easy to be handled in the upscaling process. In order to overcome the two drawbacks we developed a scale coupled multiscale upscaling model to calculate two-phase flow distributions for certain pressure in the porous plate experiment. Once the distributions are obtained the other properties, such as relative permeability and saturation factors, can be relative easily calculated by fixing the two phase boundary for capillary dominated flow. In the scale-coupled multiscale upscaling model, the geometric representation of a rock sample in certain scale is described by pores, solids and Darcy regions that have smaller under-resolved pores. Two phase flow in the pore space is directly simulated using a lattice-Boltzmann model (LBM) [2]. The two phase flow properties in a Darcy region are given by a map function. The map function can be obtained in a finer scale simulation or theoretically modeling. The map function gives the multiphase flow properties in Darcy region based on the flow phase and its pressure surrounding the Darcy region. In the meantime the boundary conditions on surface of a Darcy region of LBM simulation in resolved pores depend on two-phase properties in the Darcy region [2]. The flow distributions in pore and Darcy regions, and the boundary conditions for different scales dynamically change with applied capillary pressure (PC). The scale coupled upscaling calculation starts from the finest scale. The calculated two phase flow properties, such as PC and relative permeability, in finer scale serves as the map function of the Darcy regions in the coarser scale calculation. The upscaling completes as the calculation in the coarsest scale, usually the plug or core scale, is finished. The scale coupled upscaling of multiphase flow has been demonstrated in heterogeneous rock samples. The upscaled multiphase flow properties in different scale levels are going to be reported.

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A Speed-up Comparison of MCMC Methods for Forecasting Flows in An Oil Reservoir

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In subsurface flow prediction, uncertainty in subsurface properties plays a huge role. Markov Chain Monte Carlo (MCMC) methods are well suited for reconstructing a spatial distribution of subsurface properties. However, because of the sequential nature of MCMC, it is often impractical to use an MCMC to a problem that takes a long simulation time for a single realization. A two-stage MCMC method, in which a coarse-scale model is used to screen the proposals before running the MCMC on the fine-scale model, can be used to speed-up the MCMC simulation. This approach not only increases the speed-up, but also increases the acceptance rate. With the availability of inexpensive Graphics Processing Units (GPU's), one could also use a pre-fetch algorithm to parallelize a single MCMC chain. In this poster, we compare the two approaches in a Bayesian framework for enabling predictive simulation in an oil reservoir.

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An Efficient Multiscale Method for Two-phase Subsurface Flows

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In the numerical simulation of subsurface two-phase (water-oil) flow in petroleum reservoirs, the governing equations can be approximated by an operator splitting scheme that decouples the velocity-pressure calculation from the saturation update. We focus in the use of a multiscale mixed method to approximate velocity fields that uses the Robin boundary condition in the underlying domain decomposition of the global problem. The coupling between velocity and saturation calculations leads to the recalculation of all multiscale basis functions for each time step of the saturation transport equation. We propose a new algorithm for the velocity field calculation that replaces the update of all basis functions by the solution of one auxiliary boundary value problem in each subdomain. In parallel implementations of our method these auxiliary calculations are independent of each other, and can be computed locally. Numerical simulations are presented and discussed.

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Bayesian Methods for Seismic Inversion

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Bayesian seismic inversion can be used to sample from the posterior distribution of the velocity field, thus allowing for uncertainty quantification. However, Bayesian techniques like Markov chain Monte Carlo (McMC) can be extremely computationally expensive. We propose a two-stage McMC method where an upscaled wave equation solver is used to quickly filter out unacceptable velocity fields, thus reducing the computational expense. Our examples consider both the modeling of the velocity field within geological layers as well as the identification of boundaries between such layers. See [1] for some preliminary results of this work.

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Characterization of Rock Properties in Coupled Fluid Flow and Geomechanics Problems

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In the exploration of deep formations, alterations in pore pressure change the mechanical equilibrium of the porous medium leading to stress modifications which alter rock properties such as permeability and porosity and, consequently, the fluid flow pattern [2]. The coupling of geomechanical effects and fluid flows is widely influenced by the natural rock heterogeneity [1] and the predictability of computational models is limited by the availability of an adequate description of the formation properties, such as hydraulic conductivity, porosity, and poromechanical parameters. Since direct measurements of reservoir properties are only available at a small number of locations, the deterministic description of the hydraulic parameters cannot be accomplished at all relevant locations and alternative conceptualizations suggest that a stochastic methodology is indispensable to treat rock properties. In recent years the increase in field data acquisition (although in limited points) associated with the use of high performing computing have encouraged the use of dynamic data, such as well test data, historical pressure data, fractional flow rate, reservoir compaction and surface subsidence, directly in the simulation of processes in order to reduce uncertainties in rock properties and to improve the predictability of the models. In this work, we use the Markov-chain Monte Carlo (McMC) method to characterize the permeability, porosity and Young's modulus fields in a two-phase flow problem coupled with the geomechanics of the adjacent rocks.

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Flow Forecasting of Contaminants in An Aquifer

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In the event of an aquifer contamination we need to forecast the flow of contaminant concentration. In the flow forecasting, characterization of the aquifer subsurface is an important step. To characterize subsurface properties we use a Markov chain Monte Carlo (MCMC) algorithm. Conditioned to the data collected at monitoring wells, we use the MCMC algorithm in a Bayesian statistical description to reconstruct the spatial distribution of two important subsurface properties: permeability and porosity. By using reconstructed permeability and porosity distributions, we predict subsurface flows. In this talk, we develop a Bayesian framework for forecasting contaminants in an aquifer.

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Model Validation for Porous Media Flows

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We are concerned with the interplay between findings of laboratory experiments and model validation. We focus on a compositional two-phase flow model for the simulation of the injection of CO2 in a brine saturated core. Initially we discuss the application of the methods developed in [1] to quantify uncertainty in the three-dimensional (3D) permeability field. This process establishes the credibility of the compositional model to describe the displacement of brine by CO2. We investigate the predictive capabilities of the compositional model in the context of an unsteady-state CO2-brine drainage experiment at the laboratory scale, performed at field-scale aquifer conditions.

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Multiscale Mixed Methods for Subsurface Flow Problems

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We investigate multiscale mixed methods aiming at the efficient parallel solution of large multiphase, compositional reservoir flow problems of current interest to the oil industry.

In this presentation we will compare numerical results obtained by multiscale methods based on a Robin-type domain decomposition procedure (the MuMM, see [1]).

Initially we will present a new abstract formulation of the MuMM, written in terms of a two Lagrange multiplier field (see [3]), that avoids an iterative procedure used in [1] and allows us to define arbitrary approximation spaces on the skeleton of the domain decomposition. One can improve the accuracy of the method by using higher order interface approximations in line with the work of [2], or generalize the MuMM adopting empirical coarse-grid interface spaces [4].

We introduce a dimensionless parameter c that provides a measure of the relative importance of Neumann and Dirichlet boundary conditions within the underlying Robin condition in the definition of multiscale basis functions. Numerical results are presented and discussed, indicating that this parameter can be selected so that the MuMM solution shows improved accuracy when compared to related multiscale mixed approaches.

In Graphs 1 and 2 we exhibit the error of the MuMM with respect to the fine grid solution for two different values of c, a c value approximately zero and a value bigger then zero, respectively, in one selected layer of the SPE10 permeability field that has a strong channeling structure with a permeability contrast of Kmax/Kmin = 10^6. We consider single-phase flow with discontinuous linear spaces on the interfaces.

Our results illustrate that by a suitable choice the MuMM dimensionless parameter accuracy is indeed improved. The parameter c approximately to zero indicates dominance of the Dirichlet condition, where in the limiting case c = 0, the MuMM reduces to the MMMFEM [2].

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On the numerical simulation of the two-phase pseudo-parabolic Buckley-Leverett flow equation with heterogeneities and dynamic capillary pressure

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We present numerical approaches for solving a pseudo-parabolic partial differential equation, which models incompressible two-phase flow in porous media taking into account dynamic capillary pressure effects. In the recent past, many researchers have been worked on the causes and effects of non-uniqueness in capillary pressure and saturation relationship in porous media for transport problems in porous media with applications in oil recovery and sand-CO2-water systems under various pressure conditions aiming CO2 sequestration. These phenomena arise in a theory of two-phase flow in porous media that includes rate-dependent dynamic capillary pressure and spatial heterogeneities, then it is naturally also a multiscale problem. Indeed, a natural issue is how to correctly model the diffusion and dispersion terms driving the expected qualitative behaviour of the solutions. In this work, we briefly discuss two numerical schemes based on the operator splitting technique. Our numerical experiments show that the standard splitting, widely used to solve parabolic problems, may fail when applied to pseudo-parabolic models. Next, we present an operator splitting scheme based on a dispersive-like character that obtains correct numerical solutions. Then, we discuss an unsplit efficient numerical modelling, locally conservative by construction. This latter framework is based on a fully coupled space-time mixed hybrid finite element/volume discretization approach in order to account with efficiency for the delicate local nonlinear balance between the numerical approximations of the hyperbolic flux and the pseudo-parabolic term, but linked to a natural dispersive-like character of the full pseudo-parabolic equation. Both one-dimensional and two-dimensional problems are presented. We compare our numerical results with approximate solutions constructed with methods recently introduced in the specialized literature, in order to establish that we are computing the expected qualitative behaviour of the solutions.

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A continuous time random walk model for transport in heterogeneous porous media

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The understanding of solute transport and mixing in heterogenous porous media is fundamental for several environmental issues, including contamination, groundwater remediation and risk assessment of geological waste repositories, among others.

The intrinsic heterogenous nature of geological media, which can be observed at very different scales ranging from micro- to regional scale, gives rise to non-Fickian features that manifest themselves in the heavy-tailed breakthrough curves, as well as in the non-linear growth of the mean squared displacement and in the non-Gaussian plumes of solute particles. It has been shown that the non-Fickian character of transport is related to incomplete mixing and both phenomena are caused by the heterogeneity that modifies locally the advective-dispersive motion of solutes, as well as by the processes of mass exchange between mobile-immobile phases, such as sorption/desorption reactions.

In this work [1], we present a continuous time random walk (CTRW) model that describes the transport of solutes in d-dimensional porous media with heterogeneous advection and in presence of mobile-immobile mass transfer. These processes are taken into account by a properly defined transition times distribution, which can be decomposed into an advective and a trapping contribution. The distribution of advective transition times is obtained from the Eulerian velocity PDF [2], which in turn is derived from the conductivity distribution [3]. Trapping is represented by a compound Poisson process, in which the trapping times depend on the sorption/desorption time scale or on the diffusion times in the immobile zones. Because the advective and the trapping time scales are typically very different, we observe different temporal regimes: 1) a pre-asymptotic, advection-dominated regime; 2) a intermediate regime, in which the processes of advection and trapping compete and 3) an asymptotic, trapping-dominated regime.

We quantify the impact of advective heterogeneity and mass transfer by considering different scenarios of hydraulic conductivity and solute retention. For each case, we derive analytically the scalings of the breakthrough curves and of the moments of the particles displacements in both the pre-asymptotic and the asymptotic regimes and we study the spatial distribution of particles. Analytical results are compared with numerical particle tracking simulations in heterogeneous conductivity fields with retention.

Fig. 1 shows an example of random flow.

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Characterization of a double-continuum formulation for mixing-driven reactions through pore-scale information

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Recent advancements in pore-scale imaging techniques allow the detailed characterization of 3D porous media geometries at the pore-scale level. This information can then be employed to perform direct numerical simulation of flow, transport and reactions within pore spaces. Recent works have proposed operational procedures to employ pore-scale information into passive transport models. However, well established procedures to transfer pore-scale information to continuum-scale models are generally lacking when reactive transport processes are of concern.

We present a methodology which employs pore-scale velocity distributions to characterize the parameters of a double-continuum reactive transport model. To do this we entirely rely on the pore-scale velocity field obtained from direct numerical simulation of fluid flow within the pore space geometry obtained through imaging techniques. We focus on simple reactive setting where a mixing driven fluid-fluid bimolecular reaction takes place in the presence of advection-dominated transport, corresponding to large Péclet (Pe) and Damköhler (Da) numbers. In our proposed approach, we identify the mobile and immobile fluid regions relying on the quantification of the relative strength of advective and diffusive mass transfer processes at the pore scale. Once that the proportion between mobile and immobile regions is selected, we assume that the characteristic of the real porous domain can be mapped onto a simplified unit cell: the velocity profile characterizing the mobile region directly depends on the cumulative distribution function of the pore-scale velocity. Upon relying on such simplified unit cell we then compute the effective parameters embedded in the double continuum reactive model. We assess the ability of our reactive double continuum model through the comparison of the results yielded by the model and the direct pore-scale simulations in the same geometries. A key aspect of this contribution is that we provide an operational procedure to characterize incomplete mixing within three-dimensional pore-spaces, which typically exhibits profoundly different behavior in comparison with two-dimensional media, which are often considered as benchmark cases in the literature.

For the model assessment we consider different local and global quantities, e.g. reactant and product concentration profiles and time evolution of the global reaction rate observed in the system. Finally, the performances of our approach are critically analyzed in order to highlight strengths and weaknesses of the model presented in predicting reactive transport in both three- and two-dimensional porous media, and are also compared to other modeling approaches presented in the literature.

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Continuous time random walks for intermittent porescale particle dynamics

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We present an approach for the modeling of Lagrangian porescale velocity and acceleration time series, and the resulting stochastic particle displacements. Numerical and experimental data for porescale particle dynamics show intermittent patterns in Lagrangian velocities and accelerations, which manifest in long time intervals of low velocity and short durations of high velocities [1, 2]. This phenomenon is due to the spatial persistence of particle velocities on a characteristic heterogeneity length scale. In order to model this behavior, we focus on particle velocities sampled equidistantly along trajectories [3], which removes the intermittency observed under isochrone sampling. The space-Lagrangian velocity series is modeled as a Markov process that is continuous in distance along streamlines. It is fully parameterized in terms of the flux-weighted Eulerian velocity PDF and the characteristic pore-length. The resulting stochastic particle motion describes a continuous time random walk (CTRW). The model is applied to experimental and numerical three-dimensional porescale velocity, acceleration and displacement data.

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Direct observations of multiscale solute mixing in a microporous carbonate rock by PET imaging

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Geological porous systems exhibit heterogeneities over a wide range of length-scales that limit our current capability to accurately predict fluid transport in the subsurface. While various experimental studies on this subject are available in the literature, most of them focus on a macroscopic description of transport, e.g., by analyzing breakthrough curves (BTC) from tracer tests in reservoir core samples. Although a BTC does carry information on rock property heterogeneity at the sub-core scale, the assumption is commonly done that such heterogeneity has a uniform spatial distribution. The application of non-invasive imaging techniques (e.g., X-ray CT) has revealed that this situation is rarely encountered and that the core-to-field upscaling exercise has to be extended by a few orders of magnitude. In other words, because measurements on reservoir core samples from classic methods are inherently “effective”, they have limited predictive value. In the attempt to resolve this issue, we propose a new approach, where classic tracer tests are combined with two imaging techniques, namely X-ray and Positron Emission Tomography (PET), so as to obtain information on rock structure heterogeneity at the sub-core scale (with the former) and real-time dynamic 3D images of tracer plume migration (with the latter). We argue that the ability to directly visualize tracer concentration with such level of observational detail is key to account for heterogeneity in numerical models deterministically and the comparison with direct experimental observations provides unprecedented insight on the spreading and mixing processes in these complex systems.

A set of pulse-tracer experiments has been carried out using two distinct porous systems, i.e. a glass bead-pack and a Ketton carbonate over a wide range of Péclet numbers ($20 < Pé < 200$). During the experiments the spatial and temporal evolution of the tracer plume is imaged using [18F]PET, thus providing 3D maps of the tracer concentration distribution in the rock sample (see Figure 1). Two different numerical models are applied to describe spreading and mixing in the two systems, namely the classic ‘Fickian’ Advection Dispersion Equation (ADE) and the Multi-Rate Mass Transfer Model (MRMT), which additionally accounts for mass transfer resistances within a microporus matrix. The experiments with beadpacks confirm observations from earlier studies where homogeneous spatial and temporal spreading of the tracer has been reported. However, only few of these studies [e.g., [1] and [2]] have gathered a multidimensional data set; the results presented here are very important to “calibrate” PET imaging for sub-core scale (mm-scale) observations, in view of the inherent noise of these non-destructive techniques. Observations on the Ketton carbonate at the core-scale are basically inexistent: we observe here that -as expected- an additional mass transfer resistance is introduced by the presence of micropores (~50% of the pore space) and that this effect shows a flow-rate dependency. Most significantly, as shown in Figure 1, sub-core (1-10 mm) heterogeneities have a pronounced effect on the spreading of the tracer plume. The latter can and need to be accounted for by introducing permeability heterogeneity at the same scale [3].

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Dynamic Imaging of Reaction at Reservoir Conditions - the Impact of Chemical and Physical Heterogeneity in Carbonates

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The sequestration of carbon dioxide (CO2)—a major by-product of hydrocarbon production and use—into geologic formations is one of the long-term solutions proposed to mitigate atmospheric CO2 concentrations. The reaction taking place between CO2 dissolved in the in-situ brine and rock can result in significant changes in rock properties such as permeability and porosity. This is especially important in carbonate reservoirs where complexity in pore structure is accompanied by high fluid/solid reactivity. A good understanding of the dynamics of reactive transport at the pore scale is the first step towards predictive modelling of reactive processes during CO2 injection at the reservoir-scale. To address this, we propose an experimental method to dynamically image pore-scale reactive transport in carbonates at real subsurface conditions, representing the movement of CO2 saturated brine in the reservoir. Our main goal is to study the impact of physical and chemical heterogeneity on dissolution patterns and effective reaction rates. To achieve this, we design a 5 mm diameter by 5mm length composite core made up of calcite and dolomite, with highly contrasting reactive properties and pore structures, arranged in series. The composite core consists of Silurian Dolomite (that has a low reaction rate and highly heterogeneous pore structure) followed by Ketton limestone (calcite that has a high reaction rate and homogeneous pore structure). CO2 saturated brine (5wt% NaCl and 1wt% KCl) is flowed through the core at reservoir conditions (50°C and 10MPa) and X-ray microtomography (XMT) is used to capture the changes in pore structure induced by dissolution of the rock minerals. Direct simulation on 3D XMT images is then used to analyse the evolution of the flow properties. We find that the ratio of the effective reaction rate of calcite to that of dolomite decreases over time. This is explained through the different coupling of dynamic transport effects and reaction dynamics for the two minerals. Furthermore, evolving flow and transport heterogeneity in the heterogeneous dolomite leads to development of spatial memory effects that result in a two-stage dissolution in the calcite. The first stage is characterised by a uniform growth of channels whereby the second by the growth of a single-channel. This study demonstrates that the combined impact of pore structure and chemical heterogeneity can result in effective reaction rates different to those not dependent on these dynamic effects; this may have implications on reactive transport modelling of CO2 storage in heterogeneous carbonates.

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Dynamic simulation of pore scale reactive transport in geological porous media

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Reactive transport processes are complex in nature and currently a challenge for both experimental studies and modelling approaches. However, ongoing advances in experimental and computational technologies enable efficient dynamic simulations at the pore scale. The presented reactive transport code simulates local pore space alterations in grid-based structures at a high temporal and spatial resolution.

A workflow combining numerical solvers has been developed according to the operator splitting approach and the Lagrangian transport method. The FlowDict module of the GeoDict software package (Math2Market GmbH, Germany) iteratively computes the flow field of a given three dimensional porous geometry by applying the Navier Stokes-Brinkman equation. The AddiDict module (Math2Market GmbH) simulates the advective and diffusive motion of virtual particles. These particles carry aqueous solutions, which mix with each other and react at surfaces resulting in dissolution and/or precipitation of mineral phases at the sub-voxel scale. Kinetically controlled geochemical equilibrium calculations are performed by the C++ library of the open-source code PHREEQC (IPhreeqc, USGeneral Session ; Parkhurst & Appelo, 2013). Our code embeds the prior mentioned modules into a time loop for sequentially simulating pore-scale reactive transport. GeoDict control and data files are automatically accessed to communicate the processed geochemical data. Multiple MPI-processes are applied to provide an efficient performance of the C++ Lagrangian reactive transport code at a high temporal and spatial resolution.

Results show effects of local pore space alterations on the continuously changing hydromechanical transport parameters calculated according to the Digital Rock Physics concept (DRP). These results are compared to well-characterized experiments (e.g., Chagneau et al., 2015) validating our model and, thereby, demonstrating the efficiency of the presented code. The ongoing development of our code focuses on simulating reactive transport processes at reservoir conditions, while aiming at improving predictions at the reservoir scale due to the obtained time-resolved hydromechanical transport parameters (joint research project HyINTEGER; e.g., Henkel et al., 2016, preceding project H2STORE).

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Effect of chemical reactions on CO2 sequestration: an experimental approach

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To decrease the atmospheric concentration of CO2, sequestration techniques whereby this greenhouse gas is injected in saline aquifers present in soils are considered. Upon contact with the aquifer, the CO2 can dissolve in it and subsequently be mineralized via reactions with minerals like carbonates for instance. We investigate experimentally the influence of such reactions on the convective dissolution of CO2 by analyzing convective patterns developing when gaseous CO2 is put in contact with aqueous solutions of reactants in a confined vertical geometry. We show that the reactions can enhance convection inducing a more efficient sequestration [1,2]. In parallel, we also analyze precipitation patterns obtained when a solution of carbonate is injected into an aqueous solution of calcium ions. We show that the amount and spatio-temporal distribution of the solid calcium carbonate phase produced strongly depends on the concentrations and injection flow rate [3,4]. Emphasis will be put on the possibility to control the convective and precipitation pattern properties by varying the very nature of the chemicals. Implications on the choice of optimal sequestration sites will be discussed.

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Experimental characterization of fluid stretching in porous micromodels

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The mixing of solutes in porous media is of central importance for a range of applications, including contaminant transport and degradation, clogging in geothermal systems and CO2 sequestration. Recent stochastic theories have intended to relate the dynamics of mixing to the deformation of transported fluid elements, driven by the distributions of velocities and shear rates (e.g. Le Borgne et al. 2015). The experimental validation of these lamellar mixing theories at the pore scale requires measuring jointly the pore scale velocity fields and the statistics of Lagrangian fluid deformation. In this presentation, we discuss new results obtained from porous micromodels (de Anna et al., 2014; Gimenez et al., 2015) with different grain arrangements and pore size distributions. Using advanced image Particle Tracking techniques, we perform high resolution measurements of the distribution of pore scale deformation tensors, which govern the deformation of mixing fronts. We investigate the statistics of velocities and velocity gradients and their Lagrangian correlation. We then relate them to the rate of deformation and mixing at the macroscopic scale by comparing the elongation rates predicted from stochastic theories (Dentz et al., under review) to the experimental estimates. These results provide new insights on the upscaling of mixing processes from the pore scale fluid dynamics in porous media, and on the impact of the pore structure heterogeneity on that upscaling.

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From unstationary to stationary Lagrangian velocities in heterogeneous Darcian flow and the impact on solute dispersion

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Performing accurate preditions of transport in heterogeneous porous media is a chal- lenge because of the interplay between the spatial organization of the flow field and velocity fluctuations. Such interplay leads to transport behaviors, for instance early and late solute arrival times, which may not be predicted by advective-dispersive models for equivalent homogeneous media. Similarly, transport predictions with models based on perturbation theory remain limited to log hydraulic conductivity fields with variances smaller than 1. This study contributes to elucidating how the interplay between struc- tural properties and velocity fluctuations impacts transport processes in heterogeneous porous media. We study purely advective transport and characterize solute arrival time, dispersion and streamwise velocity distributions in heterogeneous steady Darcian flow fields with connected structures and σ2 up to 4. We show that particle velocity distri- log K butions sampled equidistantly along stream lines may be non stationary: depending on the injection mode it can evolve toward an asymptotic distribution. This spatial evolu- tion contrasts with the common assumption that ensemble average particle velocities are time independent. Further, we identify and quantify a characterisitic length scale along streamlines over wich particle velocities persist. Based on this characteristic length, we use a novel Markov-chain continuous time random walk (CTRW) model that accounts for the evolution of equidistant streamwise Lagrangian velocities as a stochastic relax- ation process (Dentz et al., 2016). We present simulation results suggesting that the CTRW model predicts reasonably well the characteristic early and late arrival times and dispersion behaviors of solute.

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Impact of compound-specific mixing and electrostatic interactions on transient transport and solute breakthrough

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Compound-specific mixing and Coulombic interactions in advection-dominated flow-through systems have been recently investigated focusing on steady-state transport and lateral mixing (e.g., [1-3]). However, the impact of these effects on transient transport and solute breakthrough has received only limited attention. In this work we present the outcomes of multitracer and multicomponent ionic transport experiments performed in saturated porous media. These bench-scale laboratory experiments were carried out in a quasi 2-D flow-through chamber, in a range of seepage velocity of 0.5-25 m/day. We used pulse injections of multiple tracers (both uncharged and ionic species) through the central inlet ports of the flow-through system. Extensive sampling and measurement of solutes' concentrations at high spatial and temporal resolution (≈1500 samples and >3000 measurements) were performed at the outlet of the flow-through setup. The experimental results show that compound-specific effects and charge-induced Coulombic interactions have a remarkable impact on transient transport not only at low but also at high flow velocities. Such effects caused a distinct behavior of measured breakthrough curves of the different solutes also at high Péclet numbers. To interpret the experimental results, we used different modeling approaches: classical advection-dispersion equation (ADE), continuous time random walk (CTRW), dual domain mass transfer equations (DDMT), and a multicomponent ionic dispersion model. The latter is a 2-D transport code [3] based on a multicomponent formulation of the electrostatic coupling between diffusive/dispersive fluxes and allowed us to capture the Coulombic effects during transport of charged species. Furthermore, we considered the flux-related dilution index as a metric of mixing and we determined experimentally its temporal profile for the different solutes measured at the outlet. This metric of mixing, used in connection with the traditional solute breakthrough curves, allowed us to distinguish between plume spreading and mixing, in particular for the cases in which this was not possible based on the sole analysis of integrated concentration breakthrough curves.

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Multidimensional Imaging and Characterisation of Buoyancy-Driven Flow in Porous Media

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The dissolution of CO2 into reservoir brines is one of the key trapping mechanisms during CO2 sequestration in deep saline aquifers. In recent years, considerable effort has been directed towards quantifying the contribution of this mechanism (referred to as 'solubility trapping') to the long-term storage capacity of a given reservoir [1]. Briefly, the dissolution of CO2 at the CO2-brine interface induces a buoyant instability in the aqueous phase following a local brine density increase in the range of 0.1-1% depending on pressure, temperature and salinity. As a result the carbon dioxide-saturated brine mixes with fresh brine up to form characteristic finger-like patterns. This downward flow pushes fresh brine to the CO2-brine interface and further enhances dissolution. This phenomenon is referred to as convective dissolution or density-driven convection (DDC).

A study has been undertaken to investigate convective dissolution in a 3D porous medium. A novel protocol is presented that uses X-ray Computed Tomography (X-ray CT) to image convective dissolution in an opaque porous medium in real time. Results are presented of experiments carried out at ambient conditions using a spherical bowl (diameter of 20 cm) that is packed with glass beads (diameter, 0.5 mm) using both homogeneous and heterogeneous configurations. In the latter case, both layered and random packing is considered. An analogue fluid pair has been devised, which possesses a maximum density differential comparable to the one observed in a supercritical CO2-brine system (about 10 kg/m3), while providing sufficient contrast for quantification by means of x-rays. During a typical experiment, scans are taken at regular time intervals for up to 6-24 hours.

The results of experiments with different packing configurations are compared in terms total flux, the dilution index, to quantify the effect of the heterogeneity. The analysis is then extended to account for the 3D nature of the system and multidimensional reconstructions of the bead pack are presented. Interestingly, it is observed that such features are not symmetric, even when the homogenous packing is considered. Results are compared to data published in the literature that include both homogeneous and heterogeneous systems. The implications associated with the presence of spatial heterogeneities affecting convective dissolution and CO2 storage in geological formations are discussed.

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Redox reactions in immiscible-fluids in porous media---Membraneless battery applications

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We create a 1.7 volt, 1/3 amp flow-battery using vanadium-zinc chemistry in two polar immiscible fluids with porous media stabilization. The immiscible fluids are salt water and methanol or ethanol. We use a porous zinc anode with a carbon-cloth current collector and a neutral electrolyte NH4Cl (MeOH) which is lighter than H2O so it sits atop the acidic salt-water cathode electrolyte which consists on Na2SO4 (aq) + H2SO4(aq) +V5+ (aq) with a graphite electrode. A neutral, non-reacting, porous medium is employed to stabilize the system. The porous zinc anode oxidizes with a -0.7 volt potential while the V5+reduces to V4+ at the cathode with a 1.0 volt potential giving a 1.7 volt battery. Current has been measured at 1 ohm resistance to be 0.3 amps. The chemistry is Anode: Zn (s) + 2(NH4Cl) – 2NH4+ - 2e-→Zn2+Cl2 in methanol Cathode: 2(VO2)+SO4 (aq)+ NaHSO4 (aq)+ 2H+ + 2e-→ 2[VO2+SO4] (aq) +H2O + NaOH (aq) The battery can be run with flowing electrolytes so charging is not necessary, or it can be run in stand-alone mode on a charge/discharge cycle.

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Rock Fracture Wall Alteration due to Mineral Dissolution: Formation of a porous altered layer and its effects on fracture flow properties

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Subsurface rock fractures act as conduits for flow in many engineered subsurface environments, such as reservoirs used in hydraulic fracturing, geologic carbon storage, natural gas storage, oil and gas extraction, and injected waste disposal. In these environments, fractures may be exposed to acidified fluids that can dissolve minerals at the fracture interface, often resulting in fracture aperture enlargement and permeability increase. This enlargement poses risks for the safe storage of fluids in subsurface reservoirs (Fitts & Peters, 2013). Although some lithologies are made up entirely of reactive minerals, such as calcite limestones, many lithologies have mixtures of reactive and insoluble minerals. For example, reactive minerals may be dispersed as large particles in a less reactive matrix or may be dispersed as a cement in the rock matrix itself. In recent studies, reactive fluids have been shown to cause preferential dissolution of the reactive phases, leaving behind a porous altered layer made up of less reactive minerals (Ellis et al., 2013; Deng et al., 2013). The growth of this altered layer has been shown to affect flow properties and limit overall fracture reactivity. In this study, we present a novel experimental setup designed to investigate reaction-induced porous altered layers and analyze their effects on fracture flow properties. The novel low-pressure reactive flow experiment is designed for flow through a simulated fraction between rectangular rock coupons, analogous to those used in shear slip experiments (Fang et al., 2016). The rock coupons measure 38 mm by 19 mm and the initial fracture was sawcut. Several different rocks, representing different mineralogies, were exposed to acidified- and near neutral brines. During flow, the pressure differential across the fracture was measured to infer fracture permeability evolution. The resulting porous altered layers at the fracture interface were examined using X-ray computed tomography imaging. Results using the Eagle Ford Shale, a layered clay-rich shale with calcite particles located in the Western Gulf Basin, show the development of a significant porous altered layer. After seven days of reactive flow, the altered layer is several millimeters wide and spans the length of the fracture. It was found that fracture apertures were enlarged only in areas where calcite nodules were present at the fracture interface (Figure 1). This layer is dominantly porous unreacted matrix, with void spaces present where calcite particles were initially present. This porous layer would present mechanical changes to the fracture interface that could affect structural integrity and slip behavior. The formation of a porous altered layer with minimal aperture enlargement presents a category of fracture alteration so far overlooked by studies of significant aperture enlargements in more homogenous model systems. Understanding the formation and effects of such a layer will be important for predicting the evolution of fracture flow and mechanical parameters in real rocks.

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Role of stagnation points in the mixing dynamics of unstable flow systems

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We study the mixing of two fluids in the presence of convective instabilities. Convection is characterized by the formation of vortices and stagnation points, where the fluid-fluid interface is stretched and compressed enhancing mixing. We consider different scenarios of increasing complexity. First, a double gyre synthetic velocity field with a single stagnation point. Second, a Rayleigh-Bénard instability in which stagnation points are located at a fixed interface. This system experiences a transition from a diffusion controlled mixing to a chaotic convection as the Rayleigh number increases. Finally, a Rayleigh-Taylor instability with a moving interface, in which mixing undergoes three different regimes: diffusive, convection dominated, and convection shutdown.

We analyze the behavior of the mixing dynamics in the different scenarios using a fluid deformation model. We show that the mixing enhancement given by the scalar dissipation rate is controlled by the equilibrium between interface compression and diffusion, which depends on the velocity field configuration. The model correctly predicts the behavior of the systems and shows that the interaction between stagnation points and the correlation structure of the velocity field is responsible for the transition to chaos of the Rayleigh-Bénard instability.

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Simulating non-Fickian transport with a correlated Taylor-Aris random walk

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Real-word transport processes in porous media are always affected by pore-scale geometry. From the Lagrangian perspective, pore-scale geometry are the reason for anomalously early or late arrival of contaminants at a control plane. In this context, anomalous refers to transport processes that go beyond macroscopic transport descriptions founded on Fickian transport laws. These transport processes are known as anomalous, pre-asymptotic or non-Fickian transport. Non-Fickianity is caused by spatial coherence in the velocity field that introduces memory and dependence into the transport process. Memory can be understood as the characteristic time particles stay within a specific velocity range. Dependence can be understood as the link between longitudinal and transversal displacement (cross-dependence) as, for instance, the direction of fast particles is often aligned with the main flow direction. Non-Fickian simulation frameworks that account for process memory exist, but the parameterization of those models (e,g,. deriving the waiting time distribution of continuous time random walk models) is often the bottleneck. We present a new PTRW framework for non-Fickian transport. Our PTRW framework contains an advection/dispersion term plus a diffusion term. By definition, diffusion is a statistically independent Gaussian process that accounts solely for the molecular diffusion. The advective term is split in two separate terms. The first term represents macroscopic advection and the second can be understood as fluctuations of velocities around the macroscopic average. In our approach, it is the second term that is designed to account for anomalous dispersion. It produces time-series of particle increments from the cumulative density function (CDF) of the velocities that are equipped with memory by enforcing that the CDF values of subsequent velocities change only slightly. This is achieved through a random walk on the axis of CDF values between 0 and 1. The physical interpretation of this concept links to the concept of Taylor-Aris dispersion. Cross-dependence is introduced by linking the absolute displacement with the deviation against the main flow direction. In diffusively dominated zones (i.e. at low absolute velocities), the deviation against main flow is totally random while particles in fast flow channels are more likely to displace along the main flow direction. We capture this link by drawing the angle against main flow from a zero-centered Gaussian distribution with a velocity-dependent variance. The whole simulation approach is controlled only by one parameter per spatial dimension. The first parameter controls the strength of memory and has a clear physical meaning as it depends on a characteristic pore-length. The other two parameter that control cross-dependence are fitting parameters. They also account for the Péclet regime. We will show that this modelling framework is capable of simulating non-Fickian transport by comparison with a pore-scale transport simulation and we analyze the approach to asymptotic behavior.

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Statistical analysis of isochrone and equidistant Lagrangian velocities for Berea sandstone: Ergodicity, Markovianity and continuous time random walks

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Understanding flow and transport at pore-scale is a key issue for the effective modeling of (anomalous) transport, mixing and reaction in porous media. However, the quantification of spatial and temporal evolution and distribution of particle velocities remains a challenge. In order to attack this problem, we simulate particle motion at pore-scale on digitized three-dimensional images of a Berea sandstone sample. Images of the rock are obtained using x-ray micro-tomography (XRMT) imaging. Image segmentation results in black and white images of the sample (1). Then Stokes flow simulations are performed using OpenFoam allowing us to obtain the velocities at the interfaces of a cubic mesh. Thus particle tracking simulations are performed based on a streamline reconstruction technique which uses the Eulerian velocity field previously obtained, based on a modified Pollock algorithm (2). Anomalous transport is investigated through breakthrough curves which exhibit early arrivals and long tailing, and in terms of the particle dispersion, which evolves with different non-Fickian scalings. These behaviors and their representation in an upscaled transport framework are analyzed in terms of the Lagrangian particle velocities measured isochronically (t-Lagrangian) and equidistantly (s-Lagrangian) along streamlines. We investigate the ergodicity of the s- and t-Lagrangian velocity series and analyze their statistical properties in terms of the velocity one- and two-point statistics. Intermittent patterns in t-Lagrangian velocity series (see Figure) are due to the persistence of low velocities over a characteristic spatial scale. This intermittency is removed in the equidistantly sampled s-Lagrangian velocity. Thus, we model the s-Lagrangian velocity series as a Markov process (3), which forms the basis of a continous time random walk (CTRW) approach for the probabilistic representation of pore-scale particle motion.

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The effect of natural groundwater flow on the dissolution of CO2 in saline aquifers

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CO2 geological sequestration is a promising technology for reducing greenhouse gas emissions based on injection of supercritical CO2 into deep saline-water aquifers. As the density of the supercritical CO2 is lower than that of the ambient groundwater, the injected CO2 is expected to accumulate above the brine and may leak back to the atmosphere in case that the sealing layer is not perfectly impermeable. However, when CO2 is dissolved in water, it becomes heavier than the CO2-free water. The situation where CO2-free water is overlaid by heavier CO2-rich water, leads to a hydrodynamic instability in which fingers of dense CO2-rich water are formed and propagate downwards, causing the CO2-free water to move upwards [1,2]. This convection process is desired as it accelerates the dissolution rate of CO2 into the aquifer water. Previous works have neglected the effect of natural groundwater flow in the aquifer and assumed it has no effect on the dissolution process. However, it was found that in some of the saline aquifers groundwater flow rate, although small, is not zero [3]. In this research, we study the effect of groundwater flow on dissolution trapping by performing laboratory experiments in a physical aquifer model using a mixture of methanol and ethylene-glycol (MEG) as a CO2 analog while varying the water horizontal flow rate. We found that water horizontal flow has a significant effect on the hydrodynamic instability and the generation of fingers. As the horizontal flow increases, the number of fingers, their wavelength and their propagation rate decrease (Figure 1). When testing high water flow rates, no fingers were developed and the dissolution process was driven by diffusion and dispersion alone. An examination of the effect of water flow on the dissolution rate revealed a complex picture. While the classic dissolution dynamic, consisting of a diffusive regime followed by a convective regime, was shown in the low water flow rates, no convection was observed in the high flow rates. It seems that several mechanisms control the dissolution rate when water horizontal flow exists. These include the unstable density-driven flow, the water horizontal flow, the mechanical dispersion and molecular diffusion. The combination of these mechanisms and the interactions between them affect the dissolution trapping in a complex non-monotonic manner and may affect dissolution trapping in flowing aquifers.

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The growth of wormholing zone in a dissolving porous medium

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At sufficiently high flow rates, the dissolution front in a porous medium becomes unstable, with a formation of localized flow paths called wormholes [1]. The dynamics of wormhole growth is highly complex, with incessant merging, fading, shielding, and tip splitting of the individual wormholes. No detailed quantitative characterization of this nonlinear dynamics has been provided yet.

In this communication, we study the growth of the wormholing zone by a combination of experimental and theoretical methods. The experimental work is performed using a simple microfluidic setup, with a gypsum block inserted in between two polycarbonate plates, dissolved by inflowing water [2]. Despite the overall chaotic character of wormhole growth (see the attached Figure), we find a number of remarkable regularities in their dynamics. First, the tip of the longest wormhole (leading edge) is advancing with a constant velocity, U. Second, the trailing sections of the interface also move with a constant velocity, V, with V<U. At the same time, the width of the wormholes increases as a square root of time. These features are reminiscent of the growth of the mixing zone in miscible displacement of a more viscous fluid by a less viscous one [3-4]. Inspired by these similarities, we have formulated a two-fluid model of the evolution of the wormholing zone, where the dissolved phase is treated as the invading fluid and undissolved phase - as the displaced fluid. The model predicts the profiles of the mean porosity (averaged along the direction transverse to the flow) which agree well with the experimental ones. These results lay the groundwork for prediction of the growth velocity of the wormholes across a variety of different system, allowing for the effective estimation of the breakthrough time, i. e. the time at which the dissolution reaches the outlet of the system. This is important for a number of engineering applications, such as dam stability assessment, leakage of sequestred CO2, and stimulation of petroleum reservoirs.

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The impact of incomplete mixing on reactive transport through heterogeneous porous media

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In reactive transport, the phenomenon of incomplete mixing has been found to reduce the rates of chemical reactions. Incomplete mixing will arise in a reactive transport system when reactions occur more quickly than mixing. This results in the formation of segregated regions of only one reactant called “islands.” These islands limit reactions, as the reactive solutes are only able to come into contact and react at the interfaces between these regions. There is a need to improve models to adequately account for the effects of incomplete mixing. This problem has been studied extensively in purely diffusive systems where incomplete mixing is found to be strong if diffusion is unable to overcome its effects. It is known that the presence of non-uniform flow fields can increase the overall mixing in a system compared to homogeneous flows where mixing occurs only by diffusion. Since non-uniform flows may enhance mixing, it is also expected that they will impact reactions. Thus, a question of interest is whether non-uniform flows will enhance or attenuate the effects of incomplete mixing. A recent study addressed this question by looking at reactive transport in a laminar pure shear flow. In this work, we develop these ideas further to examine incomplete mixing in flows that are more representative of real systems. Specifically, we study reactive transport in flows through idealized heterogeneous porous media using a Lagrangian reactive random walk algorithm. It has been observed that these systems may behave as if they were perfectly mixed due to the heterogeneity of the flow field, but with lower effective reaction rates as a result of the presence of incomplete mixing. The impact of flow deformation metrics on reactions and incomplete mixing are examined and a closure for the behavior of the mean concentration at late times is discussed.

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Towards Relating Pore-Scale Geometry with Emerging Macro-Scale Transport

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In this work [Meyer, D.W. and B. Bijeljic, Physical Review E, 2016], we attempt to directly relate the macroscopic dispersion behavior in natural porous media of different complexity with the underlying microscopic pore-space characteristics. Our effort is guided by high-fidelity pore-scale DNS of carbonate, sandstone, and bead pack samples. These samples span a wide range in terms of complexity, with comparably simple or Fickian dispersion behavior for the bead packs vs. highly anomalous dispersion for the heterogeneous carbonates. We cast the flow dynamics, that govern the advection-dominated transport process, in a form that enables a low-dimensional parametrization that is applicable for all media considered. The resulting flow and transport model reproduces the wide range of flow and transport statistics observed in the different samples. More specifically, we successfully inspect the accuracy of the model by validating the limiting dispersion behavior, the resulting velocity statistics, and also, most challenging, snapshots of tracer plumes at normalized travel times spanning several orders of magnitude.

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Upscaling of dilution and mixing using a trajectory based Spatial Markov random walk model

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The Spatial Markov Model (SMM) is an upscaled model that has been used successfully to predict effective mean transport across a broad range of hydro- logic problems. Here we propose a novel variant of the SMM, applicable to spatially periodic systems. This SSM is built using particle trajectories, rather than just travel times. By applying the proposed SMM to a simple benchmark problem we demonstrate that, like its counterparts, it can reliably predict mean effective transport, when compared to data from fully resolved direct numerical simulations. Then we propose a methodology for using this SMM framework to predict global measures of mixing and dilution, that do not just depend on mean concentrations, but are strongly impacted by subscale concentration fluctuations. In simple terms we use information from trajectories to down- scale and reconstruct approximate concentration fields from which mixing and dilution measures are then calculated. Again the comparison between measure- ments from fully resolved simulations and predictions with the SMM agree very favorably. To our knowledge this is the first time that an SMM has been applied to successfully predict mixing and dilution and presents a potentially big step forward in this arena.

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Poromechanical versus lubrication effects in flowing granular mixtures

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A recent extension of the discrete element method is reported for the simulation of dense mixtures of non-colloidal particles and viscous fluids in the non-inertial regime. As an application, we examine the interplay between rate dependent dilatancy and hydro-mechanical coupling which can be expected in debris flow. The numerical model includes sphere-sphere contacts using a soft contact approach, short range hydrodynamic interactions defined by frame-invariant expressions of forces and torques in the lubrication approximation [1], and drag forces resulting from the poromechanical coupling computed with the DEM-PFV technique [2,3]. The bulk shear stress is decomposed into contact stress and hydrodynamic stress. Statistics of microstructural variables highlight a complex interplay between solid contacts and hydrodynamic interactions. In contrast with a popular idea, the results suggest that lubrication may not necessarily reduce the contribution of contact forces to the bulk shear stress. The proposed model is general and applies directly to sheared satured granular media in which pore pressure feedback plays a key role. We argue that it can be the case for debris fow, especially during the triggering phase, when run-out include transitional phases, and when the flow is stopped.

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Rainfall induced slope failure simulations with the material point method

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Slope failures typically occur due to a change in either stress conditions or material strength that are caused by a wide range of factors, e.g. excavations, additional loading, material degradation. Rainfall induced slope collapse is a common cause of failure, where the water has the effect of decreasing the soil strength due to suction reduction and increasing the soil stresses due to the additional soil weight. An initial development in the simulation of rainfall induced failures, from failure initiation through failure evolution to the final situation is presented. The failure mechanisms are observed to be more variable than in analyses which do not consider rainfall and are often more superficial. Figure 1 shows an example analysis, where a series of superficial slides occurring at the interface between the saturated and unsaturated zones erode the slope in a retrogressive flow slide.

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Saturation influence of porous soils on slope stability

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Water saturation of porous soil leads to an imbalance of natural slopes, embankments and excavating. The first reason is an increase in load due to an increase in the unit weight of the soils inside a collapse zone. The second reason is a decrease in the soil strength due to reduced internal friction and cohesion of soils. Afterwards the resistance forces reduce because of the action of buoyancy forces in the flooding zone in the base of the slope. After that the soil subsidence changes the geometrical data and the stress-strain state of the soil in the slope. The influence of soil subsidence on slope stability is poorly understood jet. The experimental field researches and the numerical analysis were performed for evaluating these factors. The methodology of slope calculation on subsiding soils should be taken into account subsidence of base in addition to the changes in the characteristics of the soil as a result of water saturation. The executed researches showed that subsidence can have significant influence on the stress-strain state of the soil and slope stability.

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Evaluation of critical variables involved in Nanoparticles Retention during Transport in Porous Media

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The retention of nanoparticles in oil & gas reservoirs largely controls the economy injection of nanoparticles in enhanced oil recovery, wells stimulation, inhibition and remediation of formation damage by organic scales, heavy oil mobility, shift rock wettability, among other proved applications. Therefore, it is important to understand the critical variables that impact the nanoparticle retention during their transport in porous media. Numerous experiments were shown that the effluent nanoparticle concentration does not reach the injection concentration during the slug injection, indicating the existence of a retention capacity. The retention capacities depend not only on the type of nanoparticles, porous media and fluids, but also on the operating conditions, such as injection concentration and flow rate. A large penetration of nanofluids into the reservoir is required, and transport of nanoparticles is limited by the degree of retention of them in the porous medium. Therefore, the aim of this study is to investigate the impact of injection concentration and flow rate injection in the nanoparticle retention during transport in porous media through an advanced mathematical model. Mathematical functions of retention capacities of nanoparticles in porous media are developed. The functions are based on physical & chemical interaction between nanoparticles –porous matrix and reservoir fluids. The mathematical functions were implemented in a transport/retention of nanoparticles model that considers the advective and diffusive transport mechanisms. This model also accounts for nanoparticle retention and further remobilization based on a two-site model. The retention functions were coupled to a multiphase/multicomponent simulator. Besides, flow and transport equations were solved following the finite-volume method with a second-order discretization scheme. The good agreement of the simulations results with experimental observations indicates that the developed functions increases the modeling capabilities of the retention / mobilization model.The model allowsoptimizing operating conditions of nanoparticles injection in reservoirs in order to control the retained particles on the mineral surface.

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Imaged-based pore-scale modeling of fluid flow and nanoparticle transport through porous media using finite element method and Lagrangian particle tracking

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Nanoparticles (NPs) have been widely used commercially and have the potential to be extensively used in petroleum engineering as stabilizers in enhanced oil recovery operations or as tracers or sensors to detect rock and fluid properties. In this work, we describe image-based Stokes flow and nanoparticle (NP) transport through porous media modeled by finite element method (FEM) and Lagrangian particle tracking (LPT), respectively. Benefits of the FEM approach for pore-scale modeling (and particularly NP transport) include unstructured meshes, varying mesh refinement, and its ability to capture hydrodynamics close to the surface. The NP transport algorithm incorporates forces acting on the particles such as hydrodynamic drag, gravity, Brownian motion, and surface forces – specifically, tabulated surface forces can be included, which allows the use of experimental data. In addition, other relevant forces can be included if necessary. We present two x-ray computed tomography (XCT) images, a Berea sandstone and a 2.5D micromodel, that were meshed and used for image-based FEM Stokes flow modeling. Then breakthrough curves (BTCs) obtained from the NP transport model show how flow rate, surface capacity, surface forces, and surface forces mapped to XCT-image based mineralogy affect NP transport in porous media. Finally, examples of the ability to track the detailed transport of each particle through the system are shown.

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Numerical Simulation of a Polymer Gel System for In-Depth Conformance Control

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To improve the sweep efficiency in fields characterized by high water cut after production by water flooding, conformance control is required. This involves use of gels to block the high permeability or thief zones in order to divert the water into the unswept zones. In-depth placement of the gel is the primary challenge since gelation time is usually too short for the gel to penetrate deep into the reservoir. To enable this, nanotechnology has been implemented in the preparation of new gel systems. Gelation may be delayed for several weeks by encapsulation of the crosslinkers into carriers through the reservoir. Gelation occurs gradually under reservoir conditions, ensuring a controlled gel placement. The transport properties of the new gel system are currently being analyzed. To evaluate the feasibility of this system, reservoir simulation study was performed, and diversion potential of the gel system was investigated. Permeability reduction and crossflow are the main mechanisms evaluated. Permeability reduction, causing the water diversion is modelled by adsorption of the gel. Slow gelation is assumed for the kinetics model to simulate the controlled release of the crosslinkers. Velocity-dependent gelation model is also applied to improve the simulation in order to avoid gel formation around the injector. Another method proposed previously to model the in-depth gel placement is to make the viscosity of the polymer sensitive to changes in pH. The pH-sensitive polymer is then injected into the reservoir as a low-viscosity acidic fluid which will show viscosity increase when the rate-dependent geochemical reactions gradually increase the pH. Sensitivity analysis was performed on several important parameters such as injection concentration and time, and gelation rate that control the gel structure. The location of the high permeability streak is analysed to investigate gravity and crossflow. High permeability reduction in the thief zone, necessary to improve the recovery, was justified by observing the distribution of water resistance factor. Gel treatment is often efficient when there is significant permeability contrast, however, gel is not completely formed in the case of high crossflow between layers since some reactants are lost to the low permeability zone. Investigation of individual layers shows increased oil saturation and production rate of the high permeability layer which is due to the resaturation of this depleted layer. The objective of the current study is to widen the understanding of the gel system by discussing the mechanisms that control the transport of the system components and their plugging ability. Important parameters in the simulation study and challenges involved are discussed. Guidelines for selecting the best reservoir candidate and conditions of gel application are suggested.

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Numerical Simulation of particles transport and deposition in porous media at the pore scale

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Particle transport and deposition in porous media is of great importance in many practical problems including contaminant dissemination, filtration and environment issues. The objective of this study is to simulate the transport and deposition of colloidal particles at the pore scale by means of computational fluid dynamics (CFD) simulations.

The present work mainly focuses on three-dimensional numerical modeling of the process of the transport and deposition of colloidal particles in a porous medium. The medium is assumed to be modeled by a bundle of capillaries of a given radius. Thus, the pore geometry is idealized as a pipe. The velocity fields obtained by solving a hydrodynamic model composed of the Stokes and continuity equations with OpenFOAM are used as input for the particle transport model. The velocity profile is then used for a Lagrangian particle tracking process. Particle Reynolds number is assumed sufficiently small so that each particle can be considered as its center of mass moving with the fluid velocity. Moreover, particles are allowed to freely diffuse with a given diffusivity coefficient.

The considered physico-chemical conditions of the systems are such that the particle-pore wall interactions are purely attractive while the particle-particle interactions are purely repulsive. Therefore, multi layer deposition is prohibited.

The particle suspension is sufficiently dilute to consider the fluid viscosity unaffected by the presence of particles on the one hand and to justify the sequential injection of particles on the other hand. Each particle is therefore injected at a random initial position at the inlet of the pipe and its center of mass is tracked until either it reaches the outlet of the domain or it is deposited on the pore surface. Once a particle is deposited on the pore surface, a volume equivalent to that of the particle is set to be solid on the pore surface. Then the new velocity field is recalculated to take into account the influence of the presence of the deposited particle on the hydrodynamics of the flow and a new particle is injected.

For a given Peclet number, particle injection and transport processes are repeated until the evaluated probability of particle deposition tends to zero. The results have been analyzed in terms of surface coverage, permeability and porosity reduction as a function of the Peclet number. The obtained results clearly show that both deposition probability and surface coverage present two different regimes. For low Peclet numbers, or in diffusion dominant regime, they show a plateau value in accordance with theoretical predictions. For high Peclet numbers where convection is dominant, these quantities decrease with the Peclet number and the tendency will be discussed in view of available results in the literature (Veerapen et al, 2001; Lopez et al., 2004) These preliminary results need to be generalized by carrying out simulations in more complex geometries closer to real pore structures. This is an ongoing work.

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PET imaging revelas hindrance effects in MWCNT nanofluid flow

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The retention of particles in porous media is typically attributed to filtrtation effects such as straning, adsorption, or sedimentation. However, using positron emission tomography (PET) as imaging modality we were able to show the effect of hindrance in concentrated nanofluids due to particle-particle interactions. A flow-through column experiment with a MWCNT nanofluid was devised for optimal particle mobility: strong repulsive interactions between particles and between particles and the matrix (glass beads), inhibiting aggregation and adsorption and a large pore size rendering straining unlikely. Using the PET technique we could observe the transport of the MWCNT nanofluid through the glass bead packing in situ. During pulse injection of the suspension into the porous media the suspension spread out as a horizontal plume at the bottom of the column by “flooding” the respective pore volume. After this pulse injection the subsequently injected water seemed to penetrate the suspension only mobilizing MWCNTs from the top of the suspension plume rather than displacing the bulk of injected nanofluid. This mobilization from the top of the plume is most effective in the central parts of the column where the flow velocity is highest while most of the nanofluid is trapped in more stagnant zones of the pore space at the bottom edges of the column with minimal MWCNT displacement. The mobilized MWCNTs are higly diluted and only visible via the continuous diminishing of the plume from its central top boundry. These observations can be explained by a pronounced hindrance of the particle transport due to particle-particle interactions in the concentrated suspension (Lamas et al, 2012) which is only overcome at the edges of the nanofluid plume, primarily in the central zones of highest flow velocity. Controlled sedimentation experiments reveal the absence of settling for high MWCNT concentrations due to hindrance. This hindrance which inhibits gravitational settling in turn also inhibits transport, in particular at low flow velocities. In order to achieve the PET measurements the MWCNTs used in this experiment were oxidzed by oxidative acid treatment (Wang et al. 2006) and radiolabeled with the positron emitter I-125. In an uncomplicated one-pot synthesis the CNTs were labeled by an electrophilic attack of I+ on the electron-rich CNT side-wall catalyzed by the so-called iodogen 1,3,4,6-Tetrachloro-3α-6α-diphenylglucoluril (Franke and Kupsch 2010).

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Two-dimensional Modeling of Polymer Stabilized Nano-scale Zero Valent Iron Transport in Porous Media

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Nano-scale zero valent iron (nZVI) can be used to treat a wide variety of groundwater contaminants in-situ. As the bare nZVI particles have a higher tendency to agglomerate, delivery of nZVI in the subsurface to the treatment zones is challenging. Stabilization of nZVI with polymer, such as carboxymethyl cellulose (CMC) can enhance its mobility in the subsurface. This study presents numerical simulation results of a set of laboratory-scale transport experiments performed in silica sand that was uniformly packed in a glass-walled two-dimensional (2D) system to evaluate CMC stabilized nZVI transport behavior. In the transport experiments: CMC stabilized nZVI and a non-reactive dye tracer Lissamine Green B (LGB) were used; water specific discharge and CMC concentration were varied; movements of LGB, and CMC-nZVI in the sandbox were tracked using a camera, a light source and a dark box; and breakthrough curves (BTCs) of LGB, CMC, and CMC-nZVI at the sandbox outlet were analyzed. The transport experiments were simulated with a 2D multiphase flow and transport model (a compositional simulator), where LGB and CMC were considered as solutes, and nZVI was considered as a colloid. The time lapsed images from LGB dye transport experiments were used to determine the pore water velocities and media permeabilities in various layers in the sand box. These permeability values were used in the subsequent simulations of CMC-nZVI transport. The compositional simulator was modified to include colloid filtration theory (CFT) for nZVI transport, where attachment efficiency was used as a fitting parameter. The simulator also included composition dependent viscosity to account for CMC mixing. In the experiments, LGB mass recoveries were greater than 95%. The CMC mass recoveries were also greater than 95% when injected alone or with LGB, and about 65% when CMC-nZVI mixture was used. The mean residence time of CMC was significantly higher than that of LGB, and increased CMC concentration caused higher pressure drops in the sand box. Significant viscous fingering was observed when water was flushed after CMC or CMC-nZVI solution injection. The nZVI mass recovery was lower than 50% in all experiments due to attachment on the sand surfaces. The 2D simulation results were in good agreement with the experimental observations (the BTCs and plume positions of LGB, CMC, and nZVI at different times). The simulation of the experiments also provided estimation of transport parameters including attachment efficiency that can be used to predict CMC-nZVI transport in similar porous media. The simulation results imply that the compositional simulator including CFT-modified transport equations could be utilized for the estimation of CMC-stabilized nZVI transport in porous media and design of field scale implementations of CMC-nZVI for remediation.

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A discrete fracture model using a cell-centered finite volume scheme with multi-point flux approximation

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Geological porous media pose many challenges to the numerical models as one often has to deal with discontinuous full tensor permeability fields and complex geometries due to the presence of fractures in the form of e.g. joints, fissures and faults. The properties of the latter can vary substantially, e.g. they can act as preferential flow paths or barriers to flow, depending on the history of their creation. However, in many geotechnical engineering applications fractures play a very important role and their accurate description is a key quality characteristic for numerical models. Many different approaches have been developed in the past, ranging from geometrical representations of the fractures, e.g. discrete fracture models (DFM), to volume-averaged descriptions (multi-continuum models). In this contribution we want to focus on a discrete fracture model that includes the fractures as (n-1)-dimensional geometries in an n-dimensional domain. Fractures and solid matrix have individual meshes assigned to them with the restriction that the facets of the n-dimensional cells align with the (n-1)-dimensional fracture geometries. We use a cell-centered finite-volume scheme with multi-point flux approximation in both sub-domains which leads to a locally conservative scheme and an explicit evaluation of the matrix-fracture fluxes. This paves the way to an accurate modelling of non-linear multi-phase flow and transport phenomena through fractured porous media, as well as the ability to handle fractures acting as barriers to flow.

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A MPI parallel code for Discrete Fracture Network flow simulations

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Performing efficient flow simulations in fractured media represented by Discrete Fracture Networks (DFN) leads to face two main problems. First, since few deterministic information are available about underground media, the DFNs are usually generated starting from known probabilistic distributions both for hydro-geological and geometrical parameters. As a consequence, the network generated may present a rather complex geometry, with several critical features, such as trace lengths and fracture area with a multi-scale distribution, causing severe problems in building a good quality mesh conforming to the traces. The second major challenge is related to the size of the computational domain. Networks of interest for practical applications might count up to several thousands of fractures, such that a careful coding with an highly efficient handling of computational resources is mandatory.

We propose an optimization based approach in which the discrete problem can be reformulated as a quadratic programming problem with linear equality constraints, which is iteratively solved by means of a gradient based approach. We consider the flow modeled by the Darcy law, with a surrounding impervious rock matrix; the flux exchange among fractures occurs at their intersections. At each iteration of the gradient method only small independent local problems on the fractures have to be solved, requiring data on the segments of the intersecting fractures. This allows for independent meshes on each fracture not necessarily conforming to the traces and, at the same time, a natural parallel implementation of the method is possible. Our optimization method has proven to be robust with respect to severe geometrical configurations, and good scalability performances were achieved.

The parallel implementation of the method is written in C++ language, using the MPI protocol for the communication among parallel processes. The connectivity of the network and the intersections between fractures is computed in a parallel algorithm, in which the total number of operations is balanced among the total number of MPI processes. The connected graph is then split among the parallel processes using the METIS routine. The partition minimizes the number of arc-cuts and balances the estimated number of degrees of freedom (DOFs) among the sub-graphs. Recalling that only a limited number of degrees of freedom, related to the solution on the fractures intersections, need to be communicated at each iteration, we divide the parallel processes in two classes: the Masters, devoted only to the communications among processes, and the Slaves, devoted to the computations of the linear systems. Thus a Multi-Master-Slave architecture is repeated in a fractal-like structure; Master processes managing the MPI communications, Slave processes performing computations. This structure is used in order to reduce the possible communication bottleneck for large networks and strongly reduce the number of communications. To shadow the communication time, the resolution of local problems related to data resident on different processes is made before the resolution of local problems whose data are all available. The use of accelerators is actually under investigation in order to speed-up the local solution of linear systems.

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A new fracture network conform mesh used to obtain transport reference simulations

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Modeling transport and heat transfers in a fracture network remains challenging. To deal with issues like polluted groundwater, nuclear waste storage (Fourno et al. 2004), CO2 sequestration (Verscheure et al. 2012) or oil field production, this challenge have to be addressed. The geometrical complexity of a discrete fracture network (DFN) is a major issue to model transport in fractured media. The main difficulty is to build a mesh which can be used to discretize the transport equations. Recently, a new 3D DFN meshing approach was proposed. The main idea is to decompose each fracture into a number of connected closed outlines in which fractures intersections are located on their boundaries. To obtain a conform mesh, special focus is put on fracture intersections. The advantages of this mesh are to be conform and to closely respect the geometry of the DFN. The weakness is to require fine discretizations and consequently large computational costs can be expected. In the oil field context, well tests and tracer transport have to be modeled at the kilometer scale. The fractures are finely characterized on well logs and outcrops (at a scale of few meters). From this characterization a DFN can be build and may contain over 104 fractures. Due to the large number of fractures, our approach cannot be used in an industrial context. It still remains to simplify the DFN mesh, using additional assumptions about the details of the flow (Fourno et al. 2013, Khvoenkova and Delorme 2011, Noetinger and Jarrige 2011). Nevertheless, in order to test the accuracy of these assumptions, reference numerical simulations have to be carried-out using a detailed DFN geometry. This justifies using the conform mesh approach to obtain reference simulation to validate further simplifications. The presentation will explain the meshing procedure, a performance evaluation of this approach and few reference simulations obtained on different fracture networks will also be presented.

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An optimization approach for flow simulations in 3D poro-fractured media

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A novel approach for fully 3D flow simulations in fractured domains is presented. We consider a porous matrix crossed by a network of fractures, possibly intersecting each other. The fracture network is modelled by means of the Discrete Fracture Network model, and thus fractures are seen as planar polygons in the space. Flow can occur both in the fractures and in the porous matrix, and it is governed by the 3D Darcy law in the matrix and by the Darcy law on a tangential reference system on each fracture of the network. Fractures act as interfaces for the solution in the matrix, and the coupling between matrix and fractures is achieved enforcing the following conditions: continuity of the hydraulic head is prescribed at the interfaces, and the flow exiting from the matrix acts as a source term for the neighbouring fractures. Additional matching conditions prescribing continuity and balance of fluxes are imposed at the intersections between fractures. The mathematical setting of the problem consists in a large system of equations, combining the three dimensional problems in the matrix block to the two dimensional problems on the fractures and the interface conditions. Instead of solving this system of equations, the numerical solution is achieved by means of an optimization approach, in which a properly designed cost functional expressing the mismatch in the imposition of the interface conditions is minimized constrained by the equations for the Darcy law in the matrix and in the fracture planes. This formulation of the problem allows for an easy mesh generation process and for a parallel oriented approach of the flow problem in poro-fractured media. This work is a generalization of the optimization approach for networks of fractures proposed in [1,2,3,4].

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Control-Volume Distributed Multi-Point Flux Approximation (CVD-MPFA) on Unstructured Grids: Recent developments, Fracture models and Grid Constraints

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Flux-continuous finite-volume schemes are presented for flow in porous media. The schemes are control-volume distributed (CVD) with flow variables and rock properties sharing the same control-volume location and are comprised of families of multipoint flux approximations (CVD-MPFA). These schemes are designed to be consistent and flux-continuous while maintaining the reservoir simulation standard of only employing a single degree of freedom per control-volume, per flow variable, Both cell-centred and cell-vertex approximations are considered. The CVD-MPFA schemes embody a natural generalisation of the standard reservoir simulation 2-point flux scheme, and provide consistent flux approximations that extend to general tensors on structured and unstructured grids, which are consequently proving popular in reservoir simulation.

An overview of the CVD-MPFA finite-volume schemes is given for unstructured grids in two and three dimensions, which includes earlier triangle pressure support (TPS) and more recent full pressure support (FPS) schemes. Properties of the methods are presented. The FPS schemes prove to be robust for strongly anisotropic and heterogeneous permeability fields, in contrast to earlier TPS schemes. The schemes are applied to problems including fractured anisotropic media. Development of surface CVD-MPFA approximation and specific fracture model approximations are discussed. Comparisons of model performance and scheme approximation and performance are presented.

Cell-vertex approximation proves to be advantageous compared to cell-centred approximation, but requires appropriate grid types for Darcy-flux approximation, and associated grid generation issues are discussed. The methods are applied to problems involving strong full-tensor permeability fields, faults and layers. The talk will touch on a number of topics including convective (depending on time) in addition to elliptic flux approximation.

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Darcy Flow And Solute Transport In Fractured Porous Media Using Non-conforming Mixed Meshes

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Modeling subsurface water flow and transport processes in large domains has to deal with a presence of fractures and zones of preferential flow. These faults have significant impact on the transport velocity fields but are hard to resolve by the FEM methods as the width of the faults is usually of much smaller order of magnitude then the dimensions of the domain. One of possible solutions to this difficulty is to model fractures as lower dimensional objects and introduce their coupling with the surrounding continuum.

This approach assumes a computational mesh consisting of (simplicial) finite elements of different dimension called also a {\it mixed mesh}. We call the mesh conforming if its 1d elements lies on the edges of the 2d elements and these on the faces of the 3d elements, otherwise we call the mesh non-conforming or non-matching. While the discretization of the equations on the conforming grids is quite straight forward it is the meshing process which becomes hard or even fails for the dense fracture networks.

On the other hand the non-conforming meshes allow simulation on such complex geometries, but a robust algorithm is necessary for calculation of element intersections and correctly integrate communication terms between equations livind on different dimensions.

In this contribution we shall present a family of efficient algorithms for intersection of simplicial meshes and mortar like methods for coupling 1d-2d and 2d-3d mixed-hybrid finite element discretizations of Darcy flow. Further the XFEM method is employed for 1d-3d coupling in order to resolve logarithmic shape of the pressure cone. Preliminary results will be shown for the DG discretization of the solute transport on the mixed mesh.

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Discrete fracture simulation of fractured gas reservoirs: A comparative analysis of three numerical methods.

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One of the most important and complex problems in reservoir simulation is related to the fluid flow in fractured porous media. Classical continuous models of the fractured systems, such as double permeability - double porosity models, can not account for the fracture geometry and its interaction with other fractures in the reservoir. A discrete representation of the fracture systems permits the study of such variables in a reservoir. Hoverer, more complexity to the computational grid is added because the number of grids increases as well as the media heterogeneity and anisotropy. The problem lies in finding an accurate and efficient solution of the set of non-linear partial differential equations (PDE's) governing the flow in the matrix & fracture systems. In this work, we evaluate three numerical methods to solve the equations in fractured and highly anisotropic reservoirs: Unstructured finite volume method (UFVM) which is the most used method to solve transport equations, the finite element method (FEM) widely used for his flexible variational formulation, and the recently-developed Hybrid discontinuous Galerkin method (HDG) which can be seen as a combination of UFVM, FEM and classical discontinuous Galerkin method. This comparative analysis exposes the comparison between the numerical solution obtained with each of these methods showing their advantages and disadvantages in relation to geometry complexity, computational efficiency and the accuracy of the solution.

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Efficient Two-phase Compositional Flow Simulations in 2D and 3D Unstructured Gridding

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An efficient numerical model is presented that solves compositional two-phase flow in porous media with species transfer between the phases on unstructured gridding in 2D and in 3D. Our model deals with both implicit and explicit time discretization [1-3]. Implicit time discretization overcomes the severe CFL (Courant-Freidricks-Levy) condition in small grid cells. Small grid cells are required in the discretization of fractures or near well regions. Explicit time discretization is used in large matrix elements. To generate fractures in all possible orientations we have developed an interface coupled with tetgen that generates fractures as interfaces of tetrahedra elements. The implicit discretization of the species transport equation in our formulation is based on the calculation of the derivative of the molar concentration of component i in phase α (c_(α,i)) with respect to the total molar concentration (c_i). These derivatives are calculated under the conditions of constant volume V and temperature T. A combination of finite volume (FV) method and the discontinuous Galerkin (DG) method are used to discretize the mass balance equation on rectangular and triangular elements in 2D and on hexahedra, prisms and tetrahedral elements in 3D. The fluxes are calculated based on powerful features of the mixed finite element (MFE) method. Different numerical examples are presented to demonstrate the efficiency and accuracy of the model. We show that our model is stable on different types of grids in 2D rectangular and triangular elements, and in 3D hexahedron, prism and tetrahedra elements. Even in complex geometries discretized by unstructured tetrahedral elements, no convergence problems are observed.

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Fully-coupled poro-elasticity simulations on irregular grids using a black-oil flow model

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The Finite Element Method (FEM) is the favored method to solve linear elasticity not only in the manufacturing industry but also in geophysical applications. However, geological models are singular in the sense that they use irregular grids, which are necessary to capture the complexity of subsurface parameters in a compact manner. Such grids utilize cell-shapes that are not compatible with FEM discretizations. Therefore, when using FEM discretizations, re-gridding typically cannot be avoided to solve geomechanical problems. The development of Mimetic Finite Difference methods (MFD) represents a long effort to obtain discretization methods in the physical space that do not require mappings to reference element shapes as in FEM. Recently, this family of methods has been recast in the framework of FEM and, in this form, has been given the name of Virtual Element Methods (VEM). In this presentation, our goal is to show how VEM can be effectively implemented to solve, on the same irregular grid, systems coupling geomechanics and flow models that are standard in the industry. Using a flexible framework based on automatic differentiation, we implement a solver for coupled geomechanics and black-oil. We illustrate the method on realistic reservoir injection scenario.

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Hybrid discontinuous Galerkin method applied to the flow problems in highly anisotropic porous media.

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Accurate and efficient simulation of the dynamic behavior of fluid flow in highly anisotropic and heterogeneous porous media remains a challenge for the scientific and industry communities. Classical numerical methods are inefficient as fine grids are needed for dealing with step contrasts on the media and flow properties. A new conservative method, called the hybrid discontinuous Galerkin method (HDG) is presented in this work, for the numerical solution of the single-phase flow equation in porous media with complex features. The HDG is developed based on a mixed formulation of the diffusion problem using a set of equations obtained by the variational formulation. We hybridize the classical discontinuous Galerkin method weakly imposing the continuity of the normal trace of the solution. In addition, the energy conservation is accounted for in the method. The resulting method possess conservative properties with the inherited advantages of the finite element method. We analyze the performance of the method by comparing the simulation results of different porous systems with the simulation results from the finite element and volume methods. The advantages and disadvantages of the HDG method for solving flow-dynamic problems in complex porous media are discussed in terms of the heterogeneity and anisotropy.

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Large Scale Discrete Fracture Network flow and transport simulations with non-conforming meshes

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We focus on flow and transport simulations in fractured media, modeled by Discrete Fracture Networks (DFN). We consider a novel approach for simulating flow and transport in arbitrary networks stochastically generated starting from probabilistic distributions of geometrical and hydro-geological properties, with very mild constraints on the geometrical configurations and strongly relaxing any mesh generation problem. The DFN is composed by a large number of fractures, modeled as planar polygons with arbitrary spatial orientation, size and hydro-geological properties. The flow, on each fracture, is locally described by the underlying model equation. Matching conditions, ensuring hydraulic head continuity and flux conservation through fracture intersections, provide the coupling between the local problems on the fractures. In this talk we consider a novel approach proposed by the authors, in which the exact fulfillment of the matching conditions is replaced by the minimization of a proper functional, which measures the lack in continuity and flux conservation. The minimization is subject to constraints provided by the local flow or transport models on the fractures. The resulting PDE-constrained optimization problem can be discretized by FEM, XFEM or other discretization approaches without any requirement of mesh conformity at the fracture intersections. The approach has been tested both in steady-state and unsteady problems, displaying a large flexibility and reliability in several situations characterized by highly complex geometrical configurations and heterogeneous hydro-geological properties. The robustness and the efficiency of the approach allow for its application in uncertainty quantification analyses concerning geometrical and hydro-geological properties, both in steady and unsteady problems. Few enhanced models for flow and transport simulations will be considered with some practical applications to flow, geothermal and pollutant dispersion simulations.

In Figure 1 a detail of the computational mesh used for the simulation is displayed, in which the mesh non-conformities at fracture intersections are evident. In Figure 2 one of the DFNs considered is shown, counting 1425 fractures.

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Linearly Implicit Extrapolation Methods for Density Driven Flow

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Many problems in porous media science and geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases, these systems are transient and non-linear. Developing efficient solvers is a delicate task, since one needs to must combine suitable schemes for (i) time integration, (ii) linearization, and (iii) (geometric and/or algebraic) multilevel solvers, finally being employed in a (iv) parallel computing environment.

In this presentation we focus on the problem class of density-driven-flow of brine in a porous media. Previous studies, e.g. [1], investigated different non-linear solvers for this problem class. As the governing equations form a differential algebraic equation of index 1, linear implicit extrapolation methods [2, 3] are applicable. It is one striking feature of these methods, that inexact approximations of the Jacobian are admissible, when used as a so called W-method. In this presentation, we investigate different approximations and classify, which are the most favourable w.r.t. the computational effort. We present numerical experiments, report on results, and provide examples where these methods significantly improved efficiency, thus alloweing to address new sets of problems.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 365

Modeling injection induced shear failure in thermo-hydro-mechanically coupled fractured domains using an extended finite volume method (XFVM)

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A numerical approach for fractures embedded in a matrix is used to resolve shear failures in the context of an extended finite volume method (XFVM) is presented. This method for simulating mechanical failure is coupled with a hierarchical fracture model to account for flow and energy transport. The XFVM provides grid orientation independent solutions (including shear slip) without the necessity of conforming the grid around the fractures. Further, the introduction of a relaxation time scale to model the shear strength of individual fracture segments leads to converged solutions with respect to grid resolution and time step size, which is not achieved automatically. That slip solutions without this relaxation do not converge is due to the numerical failure propagation timescale introduced by the spatial and temporal discretization scales. The effects of different coupling mechanisms on this timescale is investigated, and the analysis reveals a decreasing failure propagation time scale with increasing grid resolution. On the other hand, with shear strength relaxation one obtains converged solutions including micro-seismic statistics following the Gutenberg-Richter law. Further, the sensitivity of the b-value on system parameters and boundary conditions, such as injection rate, differential stress, frictional heterogeneities etc, is investigated, and the effect of pore volume dilation on injection induced seismicity is studied.

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Nonsmooth Multigrid Methods for Phasefield Fracture Formation

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We consider a phasefield model for fracture formation in brittle materials proposed by Miehe and coworkers. Models such as this are known to allow representing advanced fracture formation and bifurcation processes. However, they are usually expensive to solve numerically, even with locally adaptive meshes. The convergence behavior of standard operator splitting techniques is not always clear. On the other hand, the solver accuracy may influence fracture dynamics.

The Miehe model describes fracture formation as the gradient flow for a system consisting of a deformation field and a scalar damage variable. Time discretization leads to a series of biconvex minimization problems. We propose a direct nonsmooth multigrid solver for the efficient and robust solution of these increment problems. This solver is a generalization of the Truncated Nonsmooth Newton Multigrid (TNNMG) method, and we prove that it converges to the solution irrespective of the initial iterate. In numerical experiments we observe multigrid convergence rates, which makes the multigrid method faster than competing algorithms.

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On the simulations of the flow in 3D fractured reservoirs

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Fluid flow simulations in the underground are particularly challenging for the nature of the subsoil that can be characterized as a porous medium crossed by a possibly intricate, multi-scale network of fractures. According to the DFN model, fractures are modelled as intersecting planar polygons, surrounded by a porous matrix. The interaction between the flow in the three dimensional matrix with the flow in the two dimensional structures representing the fractures has to be carefully taken into account in order to perform fully 3D simulations. A new approach is proposed to perform flow simulations in poro-fractured domains, based on the numerical optimization of a properly designed cost functional expressing interface conditions at both matrix-fracture interfaces and at fracture-fracture interfaces (i.e. at fracture intersections or traces, [1,2,3]). The advantages of this new method mainly consist in an easy meshing process and in a readily parallel approach. Here we focus on implementation aspects of the method and we present some numerical results obtained using standard finite elements in combination with other discretization technique, such as the boundary element method.

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Particle Decision Making Processes in Fractured Media: The War Between Models

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During a random walk through a discrete fracture network, a particle moves at a constant velocity through a fracture segment and when it arrives at a fracture intersection it chooses a path, changes velocity, and repeats the process. The set of possible velocities the particle may choose depends on which intersection it is at, inducing a correlation between its current and next velocity. This process of traveling at a constant velocity then choosing a new velocity is also a good approximation to transport in (non-fractured) porous media. For times greater than the Taylor time scale (L^2/D, where L is the length scale over which a particle must travel to sample the full range of velocities in the system and D is the diffusion coefficient), the particle's decision making process can be neglected. In fractured and highly heterogeneous porous media, however, this length scale (and time scale consequently) can be prohibitively long. Even for field scale applications, it's possible that this decision making process may not be neglected. Several upscaled models have been developed that either explicitly or implicitly model this decision making process, including continuous time random walk with a coupled space and time step distribution, the spatial Markov model, and a hybrid approach based on the Boltzmann transport equation. We ask: how do these models perform in predicting transport at scales of interest? To answer this question, we upscale transport using a variety of models in simple 2D discrete fracture networks, where transport through each fracture is purely advective (no longitudinal diffusion), yet fully mixed (infinite transverse diffusion) and there is no mass exchange between the fracture network and the rock matrix it is embedded in. This simplified testing ground reveals whether the question of "how" to model the decision process is as important as "whether" to model it. Preliminary results indicate "how" to model the process has a significant impact on model predictions.

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Projection-based Embedded Discrete Fracture Model

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Any endeavour to accurately model flow through fractured porous media at the field-scale must overcome two important challenges. First, the discretized representation of the medium needs to accommodate the complex geometry of intersecting small-scale fractures with various lengths, apertures and orientations. Second, the model formulation must ensure that the conductivity of these fractures, which can be orders of magnitude higher or lower than that of the host rock, is properly taken into account when computing the pressure map.

The Embedded Discrete Fracture Model (EDFM) [1] is well known in the literature for its flexibility in representing fractures. More specifically, in EDFM, fractures are lower-dimensional features, discretized independently from the matrix. Their effect on the flow is captured by defining fluxes between the fracture control volumes and the matrix grid cells they intersect.

EDFM was proven effective in capturing the flow behaviour through porous media containing highly conductive fractures [2,3]. However, its formulation fails to represent the effect of low-permeable features, such as embedded flow barriers (see Fig. 1). In this work, a novel projection-based Embedded Discrete Fracture Model (pEDFM) is introduced for flow simulation in fractured porous media with general conductivity contrasts [4].

Similar to EDFM, pEDFM constructs independent grids for the fracture and matrix domains. As an additional step, the transmissibilities at matrix interfaces are automatically adjusted to account for the conductivity of neighbouring fracture networks, via a scaling factor proportional to their geometric projections.

The performance of pEDFM is investigated extensively for two- and three-dimensional scenarios involving single- as well as multiphase flows. These numerical experiments are targeted at determining the sensitivity of the model towards the grid resolution, fracture position and orientation, as well as the conductivity contrast towards the matrix. The results of these studies support the conclusion that pEDFM significantly outperforms the original EDFM model and is a viable method for field-scale simulation of flow in naturally fractured reservoirs.

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Robust gridding and discretization for modelling flow in discrete facture network medium

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Subsurface geological formations are often very complex due to presence of heterogeneity and fault/fracture systems. Often modelling of fluid flow through such geologically complex fractured systems is required to model multi-physics processes like, e.g., environmental flow, CO2 sequestration, Oil and Gas flows etc. Using traditional modelling approaches, based on dual-porosity/dual permeability medium, to model such complex systems is often complicated and could result in incorrect flow patterns. Precise modelling of such complex fracture systems requires better gridding and numerical discretization techniques. In last decade alone modelling of flow through discrete fracture systems has attracted attention from a number of researchers [1, 2]. As a result few new gridding and discretization techniques have been proposed to model flow through discrete fracture network systems (DFNs). Discrete fracture networks usually involve very high or very low angle fracture-fracture intersections and sometime presence of small to very large length scale fracture networks. Numerical modelling of such a complex system is challenging, both, from gridding and numerical discretization point of view. In this paper we will present some of the advances in gridding and discretization of DFN systems, which could be potentially applied to the field of environmental flows, CO2 sequestration, and flow of oil and gas in the fractured subsurface reservoir.

In this paper we will present an in-house tool, which has been developed with advance gridding techniques to mesh complex discrete fracture network at small and very large length scales. Tool is also planned to include advance numerical discretization, and upscaling capabilities. The tool will enable modeling of geologically complex discrete fracture networks as lower dimensional objects. We will also try to demonstrate the use of the tool for modeling problems related to subsurface flows modeling in presence of complex fracture network.

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Robust simulations for uncertainty quantifications in flow and transport problems in Discrete Fracture Networks

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The effective simulation of underground flows is a challenging issue, relevant in many practical applications, such as the enhanced oil and gas production and storage, the geological disposal of pollutants or of nuclear waste, water resources management or geothermal applications. Among others, in order to correctly consider the directionality of the flows, the Discrete Fracture Network models (or DFNs) are used to provide a representation of the subsoil, that is modeled as a set of intersecting polygons, resembling the fractures in the underground, surrounded by a porous rock matrix. Being the real distribution of fractures impossible to be assessed, such networks are stochastically generated starting from probability distributions of geometrical and hydro-geological data, thus often resulting in complex geometrical domains with heterogeneous properties. From the geometrical point of view, the simultaneous presence of fractures with extremely different dimensions, spanning from few centimeters to hundreds of kilometers, or the presence of fractures intersecting with extremely narrow angles, are typical examples of computationally complex situations that might appear in DFNs for practical applications and that, combined with the large size of the domain of interest, make simulations extremely challenging. Furthermore, heterogeneity in the hydraulic properties of a single fracture and of intersecting fractures is a source of ill-conditioning for the problem. In this poster we consider a novel approach proposed by the authors in order to overcome all mesh generation problems connected to extreme geometrical complexities. The approach results to be suitable for dealing with possible very complex configurations arising from stochastic generation of the DFN. Uncertainty quantification has been applied for evaluating the effect of the variability of hydro-geological roperties in flow and transport phenomena. In Figure 1 we report a simple DFN on which we have performed an uncertainty quantification analysis for an unsteady transport problem of a passive scalar.

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Scalabilty performances for a parallel implementation in flow simulations in large scale fractured media

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We focus on efficient flow simulations in fractured media following the Discrete Fracture Network (DFN) framework. The medium is modeled as a rock matrix crossed by a network of polygonal fractures. Fractures intersect each other along segments called traces. The flow is driven by the Darcy law, the rock matrix is considered impervious, but there is flux exchange among fractures through the traces. At fractures intersections, suitable matching conditions are imposed, ensuring hydraulic head continuity and flux balance.

The DFNs are usually generated starting from known probabilistic distributions for fracture hydro-geological and geometrical parameters like position, dimensions, aspect ratio and orientation in space. As a consequence, the networks generated frequently display a complex geometry, with several critical features, such as multi-scale distribution in trace lengths and traces on fractures forming very narrow angles. These geometrical complexities may cause severe problems in building a good quality mesh conforming to the traces. By an optimization based approach, allowing for non-conforming meshes on the fractures, many of these problems could be avoided. The optimization method has proven to be robust with respect to severe geometrical configurations. A second challenge in DFN simulations is related to the size of the computational domains. Networks of interest for practical applications might count up to several thousands of fractures, such that a strongly parallel method with an efficient handling of computational resources is mandatory.

According to the optimization-based formulation, the discrete problem is reduced to several local small problems, which are iteratively solved in a gradient based method, requiring few data on the trace segments of the intersecting fractures. The parallel algorithm is written in C++ language, with a standard Finite Elements (FE) implementation, but other different discretization strategies, such as eXtended Finite Elements (XFE) and Virtual Elements (VE) can be used as a basis for the discretization. The parallel implementation described below obtains good scalability performances. The DFN is split according to a balanced partitioning among the available processes. A tailored Master-Slaves topology is devised for dealing with processes communications (Master) and computations (Slaves). This topology minimizes the number of communications, because only a limited number of degrees of freedom, related to the solution on the traces, need to be communicated at each iteration. Particular care is devoted to shadowing the communication time, postponing the resolution of local problems related to data resident on different processes, to the resolution of local problems whose data are all available. For very large DFNs the Master-Slaves structure is repeated in a self-similar structure generating a multi-Master-Slave topology.

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Schemes for Flows in Porous Media with Fractures

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In this work, we extend the single phase Darcy flow model proposed in [1], [2] to two phase flow. We thus provide a model for two phase Darcy flow through discrete fracture networks (DFN) in porous media, in which the d-1 dimensional flow in the fractures is coupled with the d dimensional flow in the matrix, leading to the so called hybrid dimensional Darcy flow model. The model accounts for fractures acting either as drains or as barriers, since it allows pressure jumps at the matrix-fracture interfaces. The model also permits to treat gravity dominated flows as well as discontinuous capillary pressure curves at the material interfaces. The discretization is based on an adaptation of the Vertex Approximate Gradient (VAG) and Hybrid Finite Volume schemes to this problem, in order to account for anisotropy and heterogeneity aspects as well as for applicability on general polyhedral meshes. The numerical analysis for the single phase flow model is carried out in an extended gradient schemes framework (see [2]). In so doing, we obtain error estimates and prove convergence, which has not been achieved before for flow in complex DFN. For two phase flow, we present several test cases including gravity and capillary effects (see Figures 1,2,3 below). The VAG scheme is used to compare our hybrid dimensional model to the hybrid dimen- sional, continuous pressure model (proposed in [3]) and to the generic equidimensional model, in which fractures have the same dimension as the matrix. This does not only provide quantitative evidence about computational gain, but also leads to deep insight about the quality of the proposed reduced model.

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Simulation of geothermal energy extraction on realistic geologies using the dual virtual element method

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Heat stored in subsurface crystalline basement rocks is a source of geothermal energy. Extraction of this energy involves circulation of a carrier fluid through naturally occurring fractures in the rock as well as through new fracturing induced by hydraulic stimulation. The network can have a highly complex geometry, with strong contrasts in conductivity and flow rates. Moreover, to simulate energy extraction, transfer of heat from the rock to water flowing through the fractures must be captured. Taken together, these effects produce a highly challenging simulation problem. Here we discuss the modeling and simulation of these processes through naturally occurring fractures, with example fracture geometries based on outcrop studies. Considering the absence of fluid flow outside the fractures, one natural modeling approach for flow is the discrete fracture network (DFN), which is built on explicit representation of all fractures. However, natural fractures occur at a continuum of length scales [1], and a simulation model including all fractures is not a practical option for energy extraction. A better suited approach is to represent small fractures by an equivalent matrix permeability, and combine this with an explicit representation of larger fractures, forming a Discrete Fracture Matrix (DFM) model. In particular, we consider a hierarchy of flow models that includes flow in the matrix (3D), in fracture planes (2D) and intersections (1D), as well as the interaction between the flow domains. To accurately represent the flow in the large fractures, they are explicitly represented in our simulation grids. The complex configuration of the network makes the gridding a challenging task, and the resulting simulation grids that can have a high number of cells. To alleviate the computational burden, we consider a grid coarsening procedure based on ideas from the algebraic multigrid literature, which produces grids of arbitrary polygonal and polyhedral shapes. On this grid, we discretize the fluid flow and heat transport using the dual formulation of the virtual element method [2], [3], which is ideally suited to handle the general grid cells produced by the coarsening. We test our approach on a case based on fracture networks observed at surface outcrops in crystalline rocks with naturally occurring fractures. The chosen field serves as an analogue for the fracture geometry in a geothermal reservoir, and contains fractures from the domain size to below the resolution of the simulation model. We study heat extraction from a 3D extrapolation of the network, with a focus on the interplay between grid resolution, simulation accuracy and computational cost.

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XFEM approximation of flow and transport in fractured porous media

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In this work we focus on a porous medium cut by a network of fractures represented as (n-1) interfaces embedded in a n dimensional domanin, with the aim of describing fluid flow and transport (advection and diffusion) in the fractures and its coupling with the surrounding matrix. We employ a method that allows for nonmatching grids, i.e. fractures can cut the background matrix and fractures cell can intersect each other. To this aim we adopt a suitable XFEM enrichment of the finite element spaces to represent possible discontinuities of the parameters and the solution at the interfaces. This geometric flexibility can be be particularly beneficial if the position of the fractures is uncertain and multiple simulations are required. The natural target applications of the proposed method is the tracking of contaminants in subsurface flows but it could be extended to deal with the simulation of geothermal reservoirs, possibly including chemical processes such as mineral dissolution/precipitation.

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3D digital core modeling and electrical simulation of natural gas hydrate

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Digital rock physics using the numerical methods to simulate the physical characteristics of pore scale, and quantitative study the relationship between rock microstructure and macroscopic properties. In order to study the relationship between the resistivity properties of the hydrate reservoir and the microstructure of the rock, and then study the change rules of the Archie's parameters and influencing factors. However, the hydrate reservoir in the terrestrial permafrost region is very dense and hard, that is to say, it's difficult to create synthetic gas hydrates in the laboratory. So, it appeared especially important to construct theoretical model. After taking the physical properties of the hydrate in the terrestrial permafrost region and its reservoir characteristics [1] into consideration, draws lessons from the ideas of constructing 3D digital cores adopt randomization method [2-3]. Then, constructing porous media model of hydrate based on the conventional digital core construction technology. In the process of model construction, a three phase porous media model consisting of rock matrix, pore water (or ice) and hydrate in fully random distribution is constructed. According to the distribution of hydrate and its reservoir characteristics. The stochastic model is improved by the corresponding constraint conditions. The porous media model with dispersed, layered, fractured and massive are constructed respectively. In the dispersion model, the hydrate is dispersed and distributed in the pore space of the rock. In the layered model, based on the actual distribution of the layered hydrate, the porous media model of the hydrate established in two forms, dispersed layer and dense layer. In the fractured model, the fractional Brownian motion model is used to construct the rough fractures with self-affine fractal features, which are superimposed on the digital cores to construct the fractured digital cores, and the hydrate is filled in the fracture space. After completing the hydrate model construction, the finite element method was used to simulate the electrical properties of the digital cores constructed above, and then analyzing the relationship between the resistivity of the natural gas hydrate reservoir and the microstructure of the rock. Consequently, the change rules of the Archie's parameters and influencing factors were obtained. In order to verify the correctness of the model constructed, a representative region was selected to obtain a set of Archie parameters by numerical simulation. After that, related data were introduced into the Archie equation to simulate the formation resistivity. Through compared the results, we can found that the results of numerical simulation and the resistivity logging curves of natural gas hydrate matched with each other well in some degree.

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A unified pore network gas flow model for shale gas applied to assess the effect of the distribution of organic and inorganic matters in gas shales on real gas flow

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A new unified pore-network gas flow model is developed to model real gas flow in a pore network that contains organic and inorganic pores and throats. It accounts for a fuller set of physical processes, including adsorption and desorption, surface diffusion, viscous flow, Knudsen diffusion in organic pore elements, whereas the viscous flow and the Knudsen diffusion in inorganic pore elements, while considering the effect of phase behavior changes in small pore elements of both types. This unified model enables an evaluation of the impact of the spatial distribution of organic matters, relative to inorganic matrix, on the gas flow. Three end-members of the spatial distribution of organic matters are considered by simulating gas flow in three pore networks that have been constructed to be representative models for each member. The pore networks contain, respectively: 1) a zone of densely connected organic pores and throats; 2) a zone of sparsely connected organic pores and throats, and 3) disconnected organic pores and throats. The results show that the connectivity of organic matters can dictate the effective gas permeability, depending on the mean radius of the organic pores/throats, relative to that of the inorganic ones. When the former is smaller than the latter, the calculated gas permeability reaches the largest and the smallest for Models 1 and 2, respectively, where the gas permeability increases more rapidly in Model 3 than the other two models when the former is greater the latter.

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An Upscaling Workflow to Predict Macro-scale Transport Properties in Gas Shales by Coupling Molecular Dynamics Simulation with Lattice Boltzmann Method

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Shale formations exhibit multi-scale geological features such as nano-pores in formation matrix and natural fractures at multiple length scales [1]. One of the key challenges in unconventional reservoir simulation is how to preserve fine-scale information in coarse-scale reservoir simulation for correct production forecasting and reserve estimation [2]. Accurate prediction of shale permeability using numerical tools requires understanding of transport mechanisms at the nano-scale, and upscaling from nano-scale to larger scale simulations. In this work, we present the coupling of the molecular dynamics (MD) simulation with the lattice Boltzmann method (LBM) on multiple-scale digital rocks, and develop an upscaling workflow that integrates nanometre-scale simulations, micrometre-scale simulations and centimetre-scale simulations. The proposed approach allows calculation of macro-scale transport properties in gas shales while significantly reducing the loss of critical fine-scale (nano-scale) information. Digital rock physics, as an alternative approach to laboratory measurement of rock/fluid properties, helps estimate shale properties for which lab measurements are difficult to achieve. Due to the limit of resolution of imaging experiments, multi-scale digital rock reconstructions are employed to depict multi-scale geological features. In the current study, we aimed to develop an integrated upscaling workflow from nanometre-scale simulations to centimetre-scale simulations with assistance of multi-level imaging techniques. In nano-scale simulations, methane transport properties in reconstructed kerogen structures and clay structures are estimated using MD simulations. The calculated methane diffusivity coefficients in kerogen are used as input parameters for LBM simulations combined with the FIB-SEM digital rock. The effective permeability of this FIB-SEM digital rock as well as clay's transport property is mapped on their corresponding voxels in Nano-CT digital rocks. Next, LBM simulations on Nano-CT digital rocks are performed to obtain the effective permeability of shale matrix at the micro-scale. Last, the effective permeability of shale matrix is mapped on the Micro-CT digital rock with the fracture network. The centimetre-scale transport property of shale can be finally estimated by the LBM simulations. In the simulation results, the effective permeability changes significantly (up to 10 times) for different shale samples. The difference in permeability is attributable mainly to porosity, organic content and fracture characteristics. It is found that the effective permeability increases when the organic content is increased, and better pore connectivity in organic matters also enhances the effective permeability. In addition, the amount, aperture and length of micro-fractures are found to have significant influences on the effective permeability.

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Analysis of thermo-diffusive cellular instabilities in continuum combustion fronts

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We explore numerically the morphological patterns of thermo-diffusive instabilities in combustion fronts with a continuum fuel source, within a range of Lewis numbers and ignition temperatures, focusing on the cellular regime. For this purpose, we generalize the recent model of Brailovsky et al. [1] to include distinct process kinetics and reactant heterogeneity. The generalized model is derived analytically and validated with other established models in the limit of infinite Lewis number for zero-order and first-order kinetics. Cellular and dendritic instabilities are found at low Lewis numbers. These are studied using a dynamic adaptive mesh refinement technique that allows very large computational domains, thus allowing us to reduce finite-size effects that can affect or even preclude the emergence of these patterns. Our numerical linear stability analysis is consistent with the analytical results of Brailovsky et al. [1]. The distinct types of dynamics found in the vicinity of the critical Lewis number, ranging from steady-state cells to continued tip-splitting and cell-merging, are well described within the framework of thermo-diffusive instabilities and are consistent with previous numerical studies. These types of dynamics are classified as “quasi-linear” and characterized by low amplitude cells that may be strongly affected by the mode selection mechanism and growth prescribed by the linear theory. Below this range of Lewis number, highly non-linear effects become prominent and large amplitude, complex cellular and seaweed dendritic morphologies emerge. The cellular patterns simulated in this work are similar to those observed in experiments of flame propagation over a bed of nano-aluminum powder burning with a counter flowing oxidizer [2]. These resemble the dendritic fingers observed in this study, in the limit of low-Lewis number (Fig. 1). It is noteworthy that the physical dimension of our computational domain is roughly close to their experimental setup.

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Challenges in Ultra-tight Rock Characterisation for Fluid Flow Modelling in Digital Core Analysis

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Ultra-tight source rocks such as shales and coals are extremely difficult to characterise due to their submicron pore sizes and complex compositions. This calls for multi-scale imaging and multi-scale characterisation. One of the key challenges in multi-scale characterisation is to establish a registration framework to allow images acquired at different field of views and resolutions to link up in order to re-construct models for subsequent modelling of physics. Due to constraints of imaging techniques, it is difficult, if not impossible, to establish a pixel-based registration framework on a fixed coordinate system. Hence, a registration framework that allows features of textures to be related to each other within the datasets would be advantageous. The authors have explored an approach based on advanced imaging processing and machine learning on a set of images of a tight rock sample, and obtained encouraging outcomes. We consider this approach applicable to multi-scale characterisation of ultra-tight source rocks too.

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Delayed adsorption/desorption-flow in shale gas production

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It is of great importance to study the dynamic gas adsorption/desorption-flow process in shale, under isothermal and constant production pressure conditions. Because organic matter (kerogen) is widely distributed in shale, it plays an important role in gas flow and adsorption/desorption. Although many mathematical models considering gas diffusion and adsorption have been proposed and evaluated, very few models consider the effect of organic matter on the dynamic, approaching equilibrium (hereinafter referred to as "delayed") adsorption/desorption process. A new experimental method has been developed for studying the delayed adsorption/desorption-flow behavior in shale gas production. The essence of the method includes accurately measuring the gas going into or coming out of a shale sample with respect to time. Dynamic gas transport process obtained from this method could be divided into two stages: the early stage dominated by the diffusion of free gas in the pores and the late stage dominated by the adsorption-diffusion for gas storage process or the desorption-diffusion for gas production process. Free gas transports firstly due to the pressure gradient, which is followed by desorption and flow of the adsorbed gas. An adsorption/desorption-diffusion (DAD) model has been developed for analyzing gas transport and storage processes in crushed particles of different sizes. The delayed effect for gas adsorption/desorption results from the dynamic mechanisms of gas dissolution and adsorption in the organic matter. The mathematical model for this phenomenon is based on dynamic adsorption/desorption experiments with a constant pressure condition. The general and approximate solutions for the DAD model have been obtained to estimate the physical parameters through a multilevel single-linkage method. Isotherm measurements for total gas and free gas reveal that the difference in gas content between total gas and adsorbed gas become greater as pressure increases. Sensitivity analyses for the model disclose that the apparent diffusion coefficient and adsorption/desorption rate coefficient determine gas transport and storage processes together. Analysis and comparison of a diffusion model, an instantaneous adsorption-diffusion (IAD) model, and the DAD model reveal that the former two models are special forms of the DAD model, and the sequence of equilibrium times required for the gas transport and storage processes is: DAD>IAD>diffusion model. The information obtained from the analysis of the experimental results includes: dynamic gas transport process, contributions of free gas and adsorbed gas to the total gas production, the apparent diffusion coefficient and the adsorption rate coefficient. A smaller adsorption rate coefficient means a greater delay effect on the gas transport process due to the adsorption/desorption-diffusion of gas in the organic matter in shale. The mathematical model can not only be applied in characterizing gas transport under laboratory conditions, but also can be applied to gas transport in shale gas reservoirs under reservoir conditions.

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Effect of CO2 Injection on micro-fracture Connectivity of High Rank Coal: compare CT images of coal samples before and after CO2 injection

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Micro-fractures are very important flow channels for coalbed methane reservoirs. However, in some of high-rank coal formation, well-developed micro-fracture systems are filled by minerals, which lead to poor pore connectivity and low coalbed methane recovery. In order to enhance the flow conductivity of coalbed methane reservoirs, carbon dioxide injection has been considered. Core flooding experiments have been conducted to compare the permeability change in previous studies. In this work, we analyze high-resolution CT images of high-rank coal samples before and after CO2 injection by applying morphological theories to study the changes of connectivity. The fracture-filling minerals are found to be calcites predominantly in our samples. Calcite-filled fractures are identified readily from CT images of samples before CO2 injection because calcites appear much brighter than the matrix, and they serve as references for comparison with those in corresponding samples after CO2 injection. In order to confirm and complement image-based comparisons, we carry out gas adsorption and pressure pulse decay tests on selected samples to derive their porosity and permeability, respectively, before and after CO2 injection. To gain evidence of CO2 and calcite reactions and their alternations to the fracture surfaces, SEM and FIB-SEM are acquired at chosen locations on selected samples based on CT image analysis. Image matching and morphological operation are carried out to quantify changes of micro-fracture connectivity. The results show that calcites exist widely in all high rank coal samples in the forms of thin layer in the preexisting penny-shape fractures prior to CO2 injection. After the injection, noticeable changes in the porosity and permeability are observed for samples with higher than lower fracture intensities. Image analysis shows that there are less calcite-filled fractures after the injection and this is supported by chemical composition change in produced fluids. At places where calcites are dissolved re-opened fractures are identified from the CT images and confirmed by SEM and FIB-SEM analysis. Moreover, connectivity is significantly changed with increase in the aperture of fracture, coordination, and surface area. The connectivity function moves to the left, which shows improvement of connectivity. This work shows evidence of CO2 injection being a plausible option of treatments for calcite-filled preexisting fractures for improving coalbed methane reservoir productions.

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Effects of transport mechanisms and properties of real gas on gas flow in organic nanoscale pores of shales – a numerical study on their relative contributions by a pore network model

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It is well-known that shale gas movement in organic nanoscale pores must be modelled by capturing gas flow behaviours in the full flow regimes, gas ad-/de-sorption and its effect on the flow, and surface diffusion, while treating real gas, PVT and viscosity, appropriately to account for the effect of confined pore space on them. So far no such a model has been developed capable of evaluating the relative contributions of each and every of those physical aspect in full on realistic organic pore space beyond just simple pores. This hinders the development of appropriate and adequate models for practical use. In this work a steady-state pore-network gas flow model that accounts for all aspects above adequately is developed to assess their contributions in organic pore space in turn. That gas flow model is applied to three pore-throat network models that are constructed from the same realistic pore network but with different mean radii at 15.6, 3.2 and 1.56 nanometres, respectively, under shale gas reservoir conditions with gas pressures ranging from 5 to 70 MPa. Results show that when average pore radius is larger than 10 nm, influences of gas property and surface diffusion on shale gas permeability are negligible. However when average pore radius is smaller than 5 nm, gas permeability is notably influenced by surface diffusion and gas properties. Furthermore when the average pore radius is less than 2 nm, gas permeability will be significantly underestimated if surface diffusion is neglected. The influence of both Tc and Pc drifting away from the expected values on shale gas permeability is negligible. Permeability sensibility analysis results based on single pore are notably different with that based on pore network model. The differences can be attributed to the fact that the mixture of large and small pores and throats under the given network connectivity in the pore networks effectively alter the characteristics of the gas permeability observed for single pores. This indicates the importance to consider spatial pore size distribution and pore connectivity when to estimate effective properties.

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Evaluation of Korteweg Shear Stresses Contribution to the Mass Flux in Micro-Nanochannels

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We revised theoretical models for predicting gas mass flow rates and pressure distributions in micro-nanochannels where rarefaction and non-continuum effects are present. The norm for obtaining theoretical predictions close to experiments in isothermal gas flow in micro-nanochannel has been to furnish the basic Navier-Stokes equation with additional terms such as first, second and higher order slip boundary conditions, diffuse volume flux and other parametric scaling. However, results do not always fully conform to experimental data over the full flow regime. Here we derived a new analytical model by considering Korteweg diffuse interface type of constitutive law for the shear stress tensor. We showed that a full Korteweg type constitutive law allows for an analytical model that gives closer agreement with experimental data over the full flow regime.

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Experimental study of shale gas production process

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Shale gas formations are complex and heterogeneous systems, with both organic and inorganic content. Shale gas is contained in porous reservoirs in three forms: free gas, adsorbed gas, and dissolved gas. A matrix pressure depletion scheme can result in pore structure deformation and permeability reduction in shale, which affects the process of gas production in shale. In this paper, shale gas production tests were carried out to investigate the effects of three different pressure depletion schemes on gas production rate and on ultimate gas recovery. The three pressure depletion schemes tested include constant production pressure, linear pressure decline, and step-wise pressure decline. Results of the gas production tests show that, for shale core samples, a production pressure depletion scheme affects not only gas production rate but also ultimate gas recovery. Pressure sensitivity of shale cores due to rapid pressure depletion caused the decrease in ultimate gas recovery. The experimental results also show that the linear pressure decline and step-wise pressure decline depletion schemes delay the permeability reduction of the shale matrix, thereby resulting in a greater ultimate gas recovery than the constant production pressure scheme in which the production pressure was dropped immediately to an end value. In the gas production tests for four shale gas core samples with the same initial gas-in-place, but to different production pressure levels, the cumulative production curves exhibited several stages, representing different gas production processes. Production of compressed free gas, adsorbed gas, and dissolved gas were identified from the slopes of the cumulative gas production versus time curves. The experimental results show that a portion of the adsorbed gas as well as a portion of the dissolved gas are not producible when the production pressure was above a certain value. The contributions of free gas, adsorbed gas, and dissolved gas to the cumulative gas production varied with the production pressure. Through the analysis of controlling factors, the free gas production has no correlation with total organic content (TOC), shale desorption properties, or stress sensitivity of permeability. At high production pressures, the adsorbed gas production is primarily affected by the shale desorption properties, while, at low production pressures, the adsorbed gas production is primarily affected by the stress sensitivity of permeability. And, although TOC can significantly increase the adsorbed gas content, the adsorbed gas production percentage of gas-in-place and TOC exhibit no correlation.

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Low Variance Gas Kinetic Particle based Solver for Simulating Shale Gas Transport in Ultra-tight Porous Media

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Scientific enquiry has aligned itself, in recent times, to the understanding of the flow physics encountered at the micro- and nano-scales. The prominence of this line of study is due to its application in the field of porous media. This work is dedicated to understanding, through simulations, the transport of shale gases in subterranean micro-porous networks which is of great significance in the oil and gas industry. The computational study of the flow in these structures is a challenge owing to the rarefied nature of the flow.

The Boltzmann equation while famous for its omnipotence across all Knudsen number regimes, is equally notorious for its formidable implementation owing to the high dimensionality of its dependent variable and the complexity of the collision operator. Though attempts made to tackle this challenge head-on have yielded significant results, the major portion of the success comes from the stochastic treatment of the equation through kinetic particle representations of which the success of Direct Simulation Monte Carlo (DSMC) is a strong testament [1]. Though potent, DSMC becomes computationally prohibitive in low signal flows owing to the large number of samples required to obtain low statistical uncertainty. This implies that the application of DSMC to study shale gas transport, which is a low signal flow, is not a recommended recourse. However, these particle methods offer a plethora of advantages, such as the natural treatment of the advection process which captures traveling discontinuities, ability to treat the whole velocity, importance sampling and amenable to a parallel implementation. It is thus, not in our best interest to write off the particle treatment prematurely.

The crux of this research is to investigate the applicability and feasibility of a solver based on a DSMC derivative method termed as Low Variance Deviational Simulation Monte Carlo (LVDSMC) [2]. The principal idea of Low Variance methods is to simulate the deviation from equilibrium exclusively. The consideration of the deviation alone leads to computational savings in the Monte Carlo evaluation of the Boltzmann collision integral. The efficiency of the method stems from the fact that this method is focused on evaluating the collision integral due to the deviation from equilibrium in low signal flows, where the deviation is small but possess critical flow information. The method, thus, maintains a constant signal to noise ratio even at low signals. In the current implementation, the linearized Boltzmann equation is assumed along with the relaxation time approximation for the collision process [3].

We try to illustrate our findings with examples which include shear-driven, pressure-driven and temperature-driven flows around arbitrary 2D shapes such as squares, cylinders, ensemble of shapes and more complex binary images of porous media. The results have been validated with literature when available and compared against other methods such as Discrete Velocity Method (DVM) and DSMC where applicable. The inference drawn from our studies suggests a strong applicability of the method to study the flow around complex geometries, however the practicability in handling cases of industrial significance is still under investigation.

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Measurements of Gas Adsorption/Desorption and Diffusion in Sub-Micron Pore of Shale

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Shale reservoir is exploited under constant reservoir temperature and down hole pressure. Besides, the gas transport mechanisms in the nano- to micro- pores are different from those of the conventional reservoirs. Therefore, it is of great importance to study the gas adsorption/desorption and diffusion process in sub-micron pore space under the reservoir conditions. Here in this study, a total of three experimental methods is discussed for the measurement of the gas transportation in sub-micron pores, including variable-volume volumetric method (VVM), constant-volume volumetric method (CVM), and pulse-decay method (PDM). The cores of the VVM include accurately measuring the volume change at constant external pressure and sustaining the system temperature. During the measurement, the pressure and temperature are acquired by the data acquisition system, and the produced gas amount is measured by a gas flowmeter in the outlet. With VVM, the dynamic gas transport process in shale is obtained. By recording the change of gas production with time, the real-time production rates will be generated for a specific temperature-pressure condition. Based on this, the process could be divided into two stages. And by combining the mathematical model for the gas transport, the apparent diffusion coefficient can be obtained. CVM is the method that is mostly used for obtaining the adsorption isotherm curve when the system volume is constant while the pressure changes. Besides, by monitoring the pressure history, the gas transport in sub-micron pore is reflected and the transport stages can be obtained accordingly. PDM is a popular method for measuring the permeability of a core and the production process while the pressure keeps decreasing. The contributions of the three different forms of gas (free gas, adsorbed gas and dissolved gas) to the ultimate gas production can be estimated by reading the production curve obtained from PDM. Experimental measurements provide a straightforward way to experimentally determine the dynamic process of gas adsorption/desorption diffusion, gas transport stages, contributions of free gas/adsorbed gas/dissolved gas and characterizing parameters (permeability and diffusion coefficient) of shale. Subsequently, new predictions of gas transport in sub-micron pore of shale could be made.

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Modelling Gas Transport in Shales

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Extraction of shale gas poses a new research challenge: understanding and quantifying the gas flow physics in exceptionally low permeability porous media with pore spaces as small as a few nano-meters across. The empirical Darcy-type models to take account of non-equilibrium effects are only heuristically extended from phenomenological models for pores with simple geometries. A pre-condition for applying these models is to simplify pore space so that the flow paths in porous media instead consist of a bundle of tortuous connected simple passages. This makes a heuristic extension of phenomenological models even more arbitrary, relying on a few tuneable parameters including the tangential momentum accommodation coefficient. To uncover the gas transport physics and to predict flow properties of porous media, we utilise high-resolution images of the pore structures of ultra-tight porous media and directly solve the gas kinetic model equations. Our findings may transform the commonly-used heuristic approaches and provide a rational scaled-up model if the sorption and surface diffusion of gas molecules can be quantitatively understood.

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Modelling the surface effect of multi-wet pores of source rocks on multiphase flow

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Modelling multiphase flow in source rocks (e.g. gas shale and coal-bed seams) has been a challenge due to their complex structures of tight pores and heterogeneous matrix mineral compositions, which give rise to complex flow behaviours. Since pores are rarely confined by sediments with a 'uniform' surface wettability, even for those formed within organic matters due to hydrocarbon generation, there is a need to understand the effect of multi-wet pores on the multiphase flow dynamics, and the impact on the prediction of macroscopic flow properties when simpler assumptions on the surface wettability are made. Moreover, conventional models of relative permeability cannot be applied to unconventional rocks without considering multi-wettability characteristics. This work uses a Rothman and Keller (RK) multiphase Lattice-Boltzmann model to study the effect of dual-wettability on gas-water flow in pores bounded by organic and inorganic minerals. Simulations were run to comprehend the physics of these processes at different saturation profiles at low capillary numbers. Results show the phase mobility and configurations are affected by different mineral configurations at submicron pores and the characteristics of phase displacements that suggest what pore filling mechanisms should be included when the effect of the dual-wettability is important.

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Molecular dynamics study of three phase coexistence hydrate system dissociation in the seafloor: the dependence on adjacent phase and cage-specific occupancy

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In order to study the microscopic mechanism for methane hydrate dissociation in the seafloor environment, build a three phase coexistence system of sea water (3.5%NaCl) + hydrate + methane gas (Fig.1). Molecular dynamics method is used to simulate the hydrate dissociation process in micro level. The dissociation of hydrate system is characterized by a diffusion of methane molecules from partially open cages at the interface, layer by layer breakdown of the hydrogen bond network of closed cages and the escape of contained methane molecules. It is found that the liquid phase and gas phase has a different effect on the rate of hydrate dissociation. At the beginning of dissociation process, the hydrate layer adjacent to liquid phase dissociated faster than layer adjacent to gas phase. But with the dissociation continued, the thickness of water film near the hydrate-liquid interface is larger than the hydrate-gas interface and pay more resistance for the methane molecules diffusion. Dissociation rate of hydrate layer adjacent to gas phase gradually exceed layer adjacent to liquid phase. The effect of fractional occupancy of large/small cage is considered in this simulation, the change of potential (Fig.2) and coordination number (Fig.3) is used to describe the dissociation rate. It is found that hydrate with similar overall occupancy differ in their dissociation behavior depending on whether the small or large cages are empty. The stability for hydrate system with empty small cages (LS) is better than the system with empty larger cages (LB). And the effect of the stability difference to hydrate dissociation rate is depending on the temperature. When the temperature is low, the hydrate system with empty large cages dissociate faster than the other system. But with temperature increased, the dissociation rate differ caused by the stability difference is decreased.

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Molecular Simulation of Competitive Adsorption between CO2 and CH4 in Shale Kerogen Spherical Nano-Pores

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Carbon dioxide is a potential fluid in shale gas exploration and development, which has been successfully applied in shale reservoir fracturing. Using carbon dioxide as a displacing fluid, as in the enhanced oil recovery (EOR) technique, in shale gas development, is attractive since such potential technique also contribute to carbon dioxide geological storage. Supercritical methane in shale gas reservoirs is either adsorbed on solid shale matrix pore surfaces or stored freely in the pore void spaces. All the shale matrix pores are in nano-scale, in which the organic kerogen pore radii are mostly less than 10 nm. The nano-scale kerogen pores provide huge specific surface area for shale reservoir. Comparing with the methane fluid stored in shale kerogen organic pores, carbon dioxide shows stronger adsorption affinity because of its intermolecular interaction with the pore surfaces. However, the adsorption/desorption and diffusion behaviors related to real shale gas productions are not well understood in such nano-confined spaces. In this work, we use Molecular Dynamics and Monte Carlo methods to model the nano-scale methane/carbon dioxide/kerogen system. Based on a novel molecular simulation workflow, the kerogen pores are constructed using Molecular Dynamics under typical reservoir condition (up to 20 MPa). The adsorption isothermal is calculated using the grand canonical Monte Carlo simulation results for a kerogen pore and fitted using competitive adsorption models. The adsorption patterns of methane/carbon dioxide mixture in the organic pores are visualized to reveal the adsorption mechanism in shale kerogen.

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New Analytical Solutions for Pressure Transient Analysis with TPG in Tight Oil Reservoirs

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In recent years, tight oil has become one of the most important global resources to explore and develop. In tight reservoir, the porosity is generally less than 10%, matrix permeability is less than 0.3 mD, and fluid flow is based on nano-scale pore throat communication system. Different from the conventional reservoirs, the obvious flow characteristics of tight formation is non-Darcy flow with threshold pressure gradient (TPG) effect. Fluid starts to flow only when the driving pressure gradient exceeds starting flow pressure gradient which is usually called threshold pressure gradient. Considering threshold pressure gradient (TPG) in tight oil reservoir, correction point source function is derived based on seepage mechanics theory, and a new well testing method with TPG is presented in tight oil reservoirs. Firstly, a point source mathematical model in infinite formation considering threshold pressure gradient is established by using Laplace transformation. Then point source solution is decomposed into two parts including point source item and additional TPG pressure drop item. Secondly, based on mirror image and principle of superposition, the pressure response of vertical well in tight oil reservoir from the effect of Darcy's flow is obtained. Finally, bottomhole pressure with TPG is solved by adding the TPG correction term. Compared with the classical analytic solution, the accuracy of new method is verified, and compared with other three methods, it demonstrates that the new method method is more accurate and easier to implement. In addition, different well types including fractured vertical well, horizontal well and fractured horizontal well with TPG effect are analyzed. The results indicate that the pressure transient curve upturns in late flow period after considering TPG and pressure derivative curve no longer shows 0.5 horizontal line during later radial flow period.

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Pore Characteristics and Controlling Factors of the Lower Cambrian Hetang Formation Shale in the Northeast of Jiangxi, China

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To identify the microscopic pore characteristics and controlling factors of Hetang Formation Shale in the Lower Yangtze Region, the pore types, pore size distribution characteristics and controlling factors of the Lower Cambrian Hetang Formation (∈1h) marine shale in the northeast of Jiangxi were analyzed by using low temperature liquid nitrogen, XRD, scanning electron microscope, mercury intrusion porosimetry, isothermal adsorption experiment and geochemical indicator test system. The results show that the pore size distribution curve of Hetang Formation Shale is characterized by “two peaks” and dominated by micropore (2nm) and mesopore (47-82nm). The hysteresis loop shows that the open parallel-plate pore and slit pores are the main pore types in shales. The pore volume of Hetang Formation Shale is only positively related to organic carbon, without obvious correlation with mineral composition and thermal evolution degree. The controlling factors of pore structure characteristics of Hetang Formation Shale are rather complicated. Further analysis shows that diagenesis and excessive thermal evolution are the two main controlling factors restricting the microscopic pore characteristics. Due to great burial depth, organic matter generates numerous micropores during pyrolysis and hydrocarbon generation, and clay minerals generate a lot of micropores and mesopores during conversion from to illite. On the other hand, the development of mesopore and macropore is far better than that of nanoscale pore, because rigid quartz mineral is the dominant composition of shale and the compaction resistance of quartz can facilitate increase of macropore volume with increase of shale burial depth. It is inferred that Hetang Formation Shale is relatively ideal horizon for developing shale gas, since the proportion of free gas is rather high and induced cracks can be generated easily, which is conductive to seepage and desorption of shale gas.

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Pore-Fracture Network of High-rank Coal Based on the Three-dimensional Digitalization Modeling

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Unlike other nations, the exploitation of coal bed methane (CBM) in China firstly obtained the success in Anthracite of the Qinshui Basin. At present, Chinese CBM is mainly produced in Anthracite reservoir. Anthracite is the tight rocks with more complex and changing pore-fracture structure and totally lower permeability. Therefore, the exploitation of CBM in Anthracite is difficult. The level of awareness of the structure and desorption-diffusion-seepage networks of anthracite reservoir is one of the key factors restricting the scientificalness of geologic evaluation and effectiveness of development technology of CBM in China. The application of Computed Tomography (CT) Images, Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM) and other new techniques make it possible for the digital characterization and three-dimensional (3D) modeling of coal reservoir pore-fracture structure in the scale of macropore and mesopores. In order to study the interconnecting characteristics of pores and fractures in high-rank coal, the study focuses on the #3 anthracite reservoir in Qinshui basin. Based on the 3D digitized modeling method of coal reservoir structure, 3D digital network model of coal bed multi-scale pore-fracture structure was established, pore-fracture parameters were extracted. Further, combined with scanning electron microscope observation, connected relations between pores and fracture and contributions of different genetic types of pores and fractures to the connectivity of coal were discussed. The results show that pore throat diameters in high-rank coal are small. Pore volume gives priority to mesopores whose diameters smaller than 50 nm. The tortuosity of pore throat is small, and pore cross-sections give priority to square and regular triangle. These mean that pore throat has small capillary pressure to gas. Pores in coal have poor connectivity. Mesopores whose diameters smaller than 50 nm are significant to the pore connectivity. There are 2 types of pores in #3 coal bed: primary pores mainly including biological structure pores and intergranular pores, and secondary pores usually including secondary gas pores, differential shrinkage pores, mineral pores and macromolecular structure pores. #3 coal bed gives priority to secondary pores. Differential shrinkage pores are the most important nanoscale interconnected pores in #3 coal bed. Due to the development of differential shrinkage pores among quartz and clay minerals of different physiochemical properties, fluid flow network structure with network topological features was formed in #3 coal bed. 3D digital network model of coal bed pore-fracture structure characterizes the distribution characteristics and topological relations of pores and fractures. It's the digital and visual characterization of the internal spatial structure of coal. Reconstruction of multi-scale and complex coal bed pore-fracture network will greatly promote the research of CBM output process and mechanism of liquid flow in coal reservoir.

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Pore-scale modelling of gas flow in porous media

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Although the unconventional gas has accounted for 67% of the natural gas resources, its production contributed only 14% of global gas supply in 2012 [1]. Understanding of gas transport in unconventional reservoirs is still challenging for experimental and theoretical studies due to its extremely small permeability and complex nanoscale geometry. To predict the gas permeability through ultra-tight porous media where the Knudsen number (Kn) is large, gas rarefaction effect which enhances permeability should be taken into account. The Darcy's law was first extended to slip regime (Kn < 0.1) in Klinkenberg model by considering the Navier-Stokes equation with gas slip on the pore surface [2]. Recently, a few models have been proposed to further expand Klinkenberg correction for all regimes by implementing the second-order slip flow boundary condition [3] or the so-called Knudsen diffusion mechanism [4]. However, these core-scale models include empirical parameters determined by fitting with numerical or experimental data. In modelling pore-scale flows, the gas kinetic theory approach is indispensable to simulate gas flow in the transitional regime (0.1 < Kn < 10). As Direct Simulation Monte Carlo (DSMC) method is extremely expensive for simulating low-speed flows in tight porous media, the kinetic model equations, which are simplified version of the Boltzmann equation, can be solved providing reliable results with reasonable computational cost. In the present work, gas flows through samples of porous media is simulated directly by solving the BGK kinetic equation [5] using Discrete Velocity Method (DVM) and Lattice Boltzmann method (LBM). The numerical data are compared with commonly used core-scale models, see Figure 1. The results show that the discrepancy between these models and the kinetic solution is small in the slip regime, and it varies in the transitional and free molecular regimes depending on the value of empirical parameters.

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Quantifying effective diffusivity of porous binder of fuel cell gas diffusion layers

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Polymer electrolyte fuel cells (PEFC) are considered as an important technology for the reduction of carbon dioxide emissions from automotive transportation. Carbon fiber based gas diffusion layers (GDL) are used in PEFCs for fine distribution of reactant gases from the flow field channels to the catalyst layer (CL). It is a key component for PEFC as it serves also for water removal from the CL as well as heat and electricity transport between CL and the flow field plates. GDL materials can be classified as woven, felts, papers, where the later type requires a binder to mechanically stabilize the fiber arrangement.

While most GDL binders are solid, the binder of SGL GDLs appears porous and it's influence on gas phase transport is unclear [1]. In SEM surface images of SGL, GDL binder domains appear as flake like fine-structure with particles of about 100 to 300 nm (see Fig. 1). Here, we apply multi-dimensional X-ray imaging techniques and multi-scale numerical simulations to clarify possible contributions of the sub-micron binder porosity to overall GDL gas transport.

The binder porosity was quantified using absorption contrast X-ray tomographic microscopy measurements at the TOMCAT beamline and ptychographic nano-CT at the cSAXS beamline of the Swiss Light Source (SLS), with voxel sizes of minimum 0.16 µm and 38 nm, respectively. Effective diffusivity of the scanned structures was calculated using the GeoDict software. In order to verify the effective diffusivity values of the high resolution tomographic datasets with limited field of view, a numerical parameter study based on ternary segmented XTM data of representative GDL samples with 2.2 µm voxel size was implemented. For this purpose the diffusivity of the binder domain was varied and the resulting effective diffusivity of the overall GDL domain was compared with experimental values, providing additional validation values for the binder effective diffusivity over larger and representative domains. The presentation will also address influences of PTFE-treatment to increase GDL hydrophobicity on pore structures and gas transport properties.

Caption Figure/Graphic 1: SGL 24 binder fine structure a) SEM image and b) X-ray tomographic microscopy with 0.16 µm voxel size.

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Study on the relationship between microscopic distribution of scattered hydrate and resistivity

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Natural gas hydrate is considered to be an important future energy resource because of its huge resource storage and clean combustion. It is widely distributed in the porous media of continental permafrost zone and deep-sea sediments. The microscopic distribution of the scattered hydrate in the pore space is very complex, may suspended in the interstitial fluid, and may contacted or cemented in the sedimentary particles[1-3]. Hydrate replace interstitial water or other fluid in the pore is a very complex process, in-pore formation of hydrate may cause pore clogging and permeability changes, and even may induce deformation of the porous media. It consequently has implications on the electrical properties, mechanical properties and others. In order to study the law of microscopic distribution and pore filling degree (ie, hydrate saturation) of the scattered hydrate effect on the rock resistivity. In this paper, four types of scattered hydrate distribution digital cores, including suspension type, contact type, cement type and mixed type, were constructed by numerical simulation technique. The change rule of resistivity under different hydrate distribution conditions was simulated by changing the pore filling degree of the hydrate. For purpose of forming an effective comparison with numerical simulation, hydrate experiments were also be carried out. Using the hydrate generation and reaction device, compatible with the center's high-resolution X-ray micro-tomography scanner, and for dynamically visualizing hydrate formation, the change law of the resistivity of hydrate core with time and the hydrate microscopic distribution images at different time were obtained. The results show that with the increase of the pore filling degree, the resistivity of four kinds of scattered hydrate distributions show a slowly increase first, then increase rapidly, and finally gradually increase and tends to stabilize. However, the resistivity curves still have obvious difference. And the mixed type hydrate distribution is in good agreement with the experimental results. According to the characteristics of the resistivity curve, a detailed analysis and study were made. It is presumed that the differences is related to the hydrate distribution in the pore space. That is, the hydrate forms in a variety of types at the same time, but as for a certain stage, some type occupies a leading position. Through this study, four different types of scattered hydrate distribution models were constructed, the variation law of the resistivity with different hydrate microscopic distribution and the pore filling degree was obtained, and the change law of resistivity was analyzed. The specific details research will be continue in the future. In addition, the theoretical model constructed make up for the insufficient of quasi-static observation in experiment, playing an important role in study the hydrate microscopic distribution and pore filling degree effect on the electrical, mechanics and other characteristic.

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Electro-osmosis in inhomogeneously charged microporous media by pore-scale modeling

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Surface charge at solid-electrolyte interface is generally coupled with the local electrolyte properties (ionic concentration, pH, etc.), and therefore not as assumed homogeneous on the solid surfaces in the previous studies. The inhomogeneous charge brings huge challenges in predictions of electro-osmotic transport and has never been well studied. In this work, we first propose a classification of electro-osmosis based on a dimensionless number which is the ratio of the Debye length to the characteristic pore size. In the limit of thin electrical double layer, we establish a pore-scale numerical model for inhomogeneously charged electro-osmosis including four ions: Na+,Cl-,H+ and OH-. Based on reconstructed porous media, we simulate the electro-osmosis with inhomogeneous charge using lattice Boltzmann method. The nonlinear response of electro-osmotic velocity to applied electrical field and the reverse flow have been observed and analyzed.

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Implementation of cement paste pore system to simulate autogenous self-healing with Lattice Boltzmann method

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Concrete is the most widely used man-made material. The main components of concrete are cement paste, aggregates and water. As binder in concrete, cement paste mainly consists of unhydrated cement, hydration products (mainly calcium silicate hydrates (C-S-H) and calcium hydroxide (CH)) , water and pores. In general, there are two kinds of pores exist in cement paste, namely, capillary pores and gel pores. The capillary pores form because the hydration products do not fill all the space between formed products. The capillary pores vary in shape and form an interconnected system randomly distributed throughout the cement paste. The gel pores are an intrinsic part of the C-S-H. The gel pores is less than 2 or 3 nm in nominal diameter, while capillary pores range from hundreds nanometers to a few micrometers [1]. The movement of liquid water and dissolved ions in cement paste is attributed to the pore system shown in Fig. 1 [2]. Furthermore, microcracks are inevitable during the curing stage and the service period of the concrete structure. The cracks range from a few micrometers to hundreds of micrometers.

The influence of (micro)cracks on the performance of concrete structures is complicated. On the one hand, the microcracks are the preferential ingression channels for aggressive ions, e.g., chloride, sulphate, etc. On the other hand, the microcracks have potentials to self-heal autogenously due to the continuous hydration of unhydrated cement and carbonisation. The autogenous self-healing involve a series of chemical and physical process of including dissolution of unhydrated cement particles, transport of ions via pore system, nucleation of hydration products and carbonization product within the cracks, as shown in Fig. 2. The complicated process of autogenous self-healing, however, can be described by numerical simulation models.

The aim of this paper is to simulate the chemical and physical process of autogenous self-healing of cement paste with Lattice Boltzmann method (LBM). Because of the large size range of pores and microcrack, it is not efficient to implement cement paste as a typical porous media [3]. However, the effective diffusion coefficient can describe the diffusion through the pore space of porous media, and the porosity is proportional to the effective diffusion coefficient [4]. The effective diffusion coefficient of each phase is used to represent different phases. In the simulation process, the dynamic diffusion coefficient of solid phases is coupled with the phase change, due to the dissolution and nucleation. The influences of this process on the stability and accuracy in LB model is explicitly studied in this paper. The result indicates that the relaxation time and the ratio of high and low diffusion coefficients play vital roles for satisfactory results.

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Lattice Boltzmann method

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Microfluidic devices have drawn a lot of interest in biotechnology, where they can be used e.g. to separate platelets, white blood cells and red blood cells, or to detect macromolecules such as DNA. Nanopore-based and nanofluidic technologies seem to offer a good potential for high-throughput and affordable DNA sequencing [1] or for clean energy generation and water purification/desalination. Such applications involve complex flows under confinement, possibly with electrokinetic phenomena (coupled electrostatic and hydrodynamic effects). It is therefore important, in order to design setups or analyze experimental results, to be able to simulate such flows. Nevertheless, artefacts may arise due to the finite size of simulation boxes [2, 3]. In particular, Yeh and Hummer have shown that hydrodynamic effects lead to systematic size-dependent corrections to the diffusion coefficient (or mobility) in molecular simulations.

Here we use the Lattice-Boltzmann method (LBM) [4] to investigate systematically the effect of the simulation box size and shape on the hydrodynamic flow generated by a point force in a bulk fluid (with an appropriate background compensating force), which corresponds to the Green's function for the Navier-Stokes equation. We show that the LBM is able to correctly predict the resulting finite-size correction on the mobility, both for cubic and anisotropic simulation boxes. In addition, we show that the results can be analyzed within the framework of linear-response theory to compute the velocity auto-correlation function (VACF) of a tracer particle. The long-time tail of the VACF predicted by hydrodynamic theory [5] is indeed observed for large simulation boxes, but is followed an exponential regime due to the finite box size. This demonstration of feasibility in bulk systems opens the way to the systematic study of finite-size effects on the mobility of confined fluids.

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Lattice Boltzmann Methods for flow dynamics and mass transport in porous electrodes

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Recent technologies provide new techniques to produce innovative fibrous porous materials which can be efficiently used in industrial energy applications [1], e.g. electrodes in fuel cells (FC) and in other energy conversion and storage systems such as Redox Flow Batteries (RFB) [2]. In FCs the performance should be largely improved designing a porous media able to efficiently transport away the liquid water phase forming at the cathode [3]. In RFB is instead necessary to enhance the slow mixing through the fibrous electrode of the reacting species dispersed in liquid acid solutions. In both cases the bottleneck of the peak performance is caused by a mass transport loss which could be reduced using optimal microstructure of the porous electrodes. The present study aims to provide a numerical tool based on the Lattice-Boltzmann Method to simulate the flow behavior in the microscopic complex pores constituting the reacting electrodes of FCs and RFBs. A two-phase thermally-coupled Lattice-Boltzmann model has been coupled with an efficient bounce-back algorithm in order to accurately solve the flow through the fibers composing the porous medium. The developed numerical tool has been applied considering a single-phase flow in a fibrous electrodes as a model of a RFB determining the mass and momentum transport properties varying the typical orientation of the fibers. The analysis shows that electrodes with fibers preferentially oriented with the flow has the lowest momentum losses compared with isotropic media, still maintaining the same levels of dispersions [4]. The numerical tool considering two-phase conditions has been applied to fibrous electrodes which mimics FC electrodes. In this case, porous media characterized by different wettability features, hydrophilic and hydrophobic, shows the best performances to efficiently transport the liquid water. A description of the tool and its application to energy conversion and storage systems will be presented in the paper.

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Lattice-Boltzmann simulations to investigate the pore-fluid contributions to the net Darcy flux

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Investigations revealed significantly variable flow patterns, varying from most tortuos, vortical flow to most straight, chanellized flow, from the beginning to the end of Darcy range. Despite the variable flow patterns in mico-scale, the macroscopic characteristics, i.e variation of flow rate and pressure difference satisfied the Darcy law. We specially investigated the share of pores to the net flux, i.e the flow that passes through the medium. The study was performed firstly using the analysis of streamlines. The streamlines calculated over the velocity fields were analysed to identify those belonging to the net flow. Other streamlines with comparatively large pathlines and rotating behaviour were recognised as those belonging to vortices. Based on the results, vortices were identified, mostly in lower macroscopic velocities, with no share to the net flow. Other classical methods for vortex identification (Q, Delta and Lambda-2 methods) using the velocity field were also employed to distinguish the vortices. The remaining flow regions were identified as net flow streams. Both methods integrated together proved a variable volume of pore space contributing to the net flux. The share of pores to the net flow enlarges throughout the Darcy regime, from a small portion of pore space (in the shape of narrow stream fingers) to almost whole the pores, from beginning to the end of the Darcy range. The uncovered vortical regions could have a significant impact on the transport properties of the porous media.

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Reactive transport modelling of pore-size dependent mineral dissolution and precipitation

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Precipitation and dissolution reactions in porous media dominate and control a large number of geochemical processes and industrial applications that span from geothermal energy and georesources to pharmaceutical products, batteries, catalysts and to long-term nuclear waste containment. The precipitation-dissolution of minerals from aqueous solutions alters the pore space and its connectivity in a way that has a complex feedback to the ion transport in aqueous phase itself. Fundamental in-depth understanding and accurate prediction of the underlying processes can be enhanced by direct pore-scale modeling, e.g. by the lattice Boltzmann (LB) method, supported by experimental investigations.

The LB algorithms are based upon the solution of the Boltzmann BGK equation on a square/cubic lattice discretized space. The kinetic origin, the statistical description of particle populations and the locality of the numerical operations facilitate the modeling and simulation of transport phenomena in realistic complex geometries at the microscopic scale, as depicted e.g. by X-ray tomography imaging of porous media with resolution down to 20nm [1]. Evolution of permeability and effective diffusivity can be determined exactly using the lattice Boltzmann modeling framework, in order to pass information to the macroscopic solvers.

In this contribution we present the results of reactive transport LB calculations aiming at reproducing a well-defined reactive transport experiment [2], in which BaCl2 solution was introduced in a porous system consisting of a reactive celestite layer embedded in quartz sand, producing extensive barite precipitation. Chemical composition and mineralogy of the samples had been previously analyzed at the microscale using synchrotron-based X-ray techniques at the Swiss Light Source, SLS at PSI. The LB algorithm was coupled with classical nucleation theory to describe homogeneous and heterogeneous precipitation of barite. Sub-lattice modelling of nucleation kinetics allowed correlating the induction time for the formation of first critical nuclei with the degree of supersaturation. The strong dependence of nuclei formation on pore size could also be taken into account. Moreover, a model for the reactive surface area for homogeneous nucleation was also implemented, setting the pace of precipitation.

The comparison of experimental and modeling results clearly shows the benefits of this pore-level modeling approach, in spite of some limitations.

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Simulation of Shale-Proppant-Fluid Interaction in Hydraulic Fracturing by Coupled LBM-IBM-DEM Scheme

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The purpose of this study is to introduce a feasible computational framework for simulating the interactions between shale, proppant and fracturing fluid and to investigate micromechanisms of proppant transport, fluid leak-off, fracturing width evolution, etc. The numerical results are of great help to the design of fracturing process and proppant placement in oil and gas reservoirs.

The LBGK scheme with a forcing term of the lattice Boltzmann method (LBM) is employed to solve the Newtonian fluid flow. The discrete element method (DEM) is adopted to handle the interactions of proppant particles and the adhesive bond of rock particles. The rock motion and fracturing can be represented by the movement of particles and the rupture of inter-particle adhesive bonds. An iterative version of boundary-condition enforced immersed boundary method (IBM) is introduced to calculate the hydrodynamic force between moving proppant particles and the surrounding fluid. Some efforts are made to improve the numerical stability and accuracy. Besides, the coupled LBM-IBM-DEM algorithm is parallelized to enhance the computational efficiency.

Several numerical examples have been set up to testify the model's capability to demonstrate the micromechanism of proppant transport and proppant-fluid-rock interactions in a coupled way. Moreover, different categories of parameters, for instance, fluid properties, proppant attributes, shale characteristics and fracturing implementation, were adjusted separately or jointly to show their influences in the fracturing effect. Also, the rock erosion occurred during fracturing was modeled and observed directly and its influence was quantified.

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Yantra: A lattice Boltzmann Method based tool for multiscale/multiphysics simulations

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Modelling of coupled physicochemical processes at different scales is important for varieties of applications related to porous media such as chemical degradation of cementitious materials, transport and sorption of contaminants, environmental contaminant transport, bioremediation or geologic sequestration of carbon dioxide. Development and applications of such models involves description of pore structures at each scales and use of simulation tools which are able to model physicochemical processes at required scales. This poster introduces a newly developed simulation tool called Yantra [1] based on lattice Boltzmann method which is able to simulate coupled processes in complex porous systems. Yantra follows a three level implementation structure to provide ease of use for the user and at the same time to be highly performant. Lowest level is a solver layer which is implemented in high performance language such as FORTRAN or C++. The solver layer needs one time compilation during the installation. Modules which assure the communication of different solvers and between different components of model with which user can interact are implemented in Python. This layer is the model component layer. User defined models can be derived by special tools which are provided within the model component layer. Currently available modules in Yantra are advection-diffusion and reactive transport module. The next version will include fluid flow and multiphase flow solvers. The solver layer is implemented for two types of scales viz., the pore scale with solid (non-diffusive) and pore spaces and the multi-level pore scale with non-diffusive solids. The lattice Boltzmann transport solver in Yantra has been coupled with geochemical solver PHREEQC [2] which allows accounting for a wide range of geochemical reaction network through thermodynamic databases. Special attention has been devoted to high computational performance of Yantra by careful algorithm optimization and parallelization using openMP.

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Algebraic Dynamic Multilevel (ADM) method for simulations of flow in porous media in presence of complex physics

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Simulations of multicomponent multiphase flow in porous media in presence of complex physics (e.g., capillarity, phase behavior, chemical reactions) require high resolution grids to accurately capture all interactions without depending on averaged (upscaled) quantities. The size of natural formations make simulations with high resolution grids impractical with today's computational power. In addition, reservoir heterogeneity is described with high resolutions, with no separation of scales. To resolve this challenge, an Algebraic Dynamic Multilevel (ADM) method [1] for fully-implicit simulations is proposed. The governing equations are discretized with a fully-implicit (or sequential implicit) method on a fine-scale grid that has the resolution required to accurately capture all physical interactions and heterogeneity. ADM maps the fine-scale Jacobian to a dynamically defined multilevel grid of nested topology. The appropriate grid resolution is employed in each part of the domain so that all interactions are captured at their proper length-scale. The mapping between the different grid resolutions is done by the means of sequences of restriction and prolongation (interpolation) operators. Finite-volume restriction operators are used, so that mass conservation is ensured, whereas different type of prolongation operators are considered. The ADM method is applied to challenging 2D and 3D heterogeneous test cases involving highly non-linear physics. It is shown that ADM provides accurate solution by employing only a fraction of the fine-scale grid cells.

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Algebraic Dynamic Multilevel Method for Flow in Heterogeneous Fractured Porous Media (F-ADM)

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We present an Algebraic Dynamic Multilevel method for flow in heterogeneous porous media with embedded discrete Fractures (F-ADM). The fully (or sequential) implicit system for the fractured formation is described on a dynamic multi-level nested grid, for both fractures and matrix [1]. The grid resolution is obtained on the basis of an error criterion, independently for each medium. Once the multilevel grids are defined [2], F-ADM employs sequences of restriction and prolongation operators to the fracture-matrix coupled fine-scale system. The prolongation operators map the solution of each medium (fracture and matrix) at resolution i to a finer one at level j, for which several choices of constant, bilinear, and multiscale basis functions are considered. Sets of restriction operators are constructed based on the finite-volume method, to ensure mass conservation at all levels. Systematic numerical test cases for heterogeneous fractured reservoirs are presented, including realistic maps from geological outcrops. For these cases, the accuracy and applicability of F-ADM is verified. It is shown that F-ADM provides accurate solutions by employing only a fraction of the fine resolution grid-cells. As an advantage to the existing Dynamic Local Grid Refinement (DLGR) methods, it is purely algebraic and applicable to complex fractured media with heterogeneous rock properties, without requiring upscaled quantities. As such, F-ADM is a significant step forward in the application of multilevel methods for naturally fractured media.

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Eigenvector centrality for topological characterization of porous media

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Predictability of flow and solute transport in porous media remains challenging. This type of calculations usually involve the solution of a system of discretized differential equations which could lead to extreme computational complexity depending on the accuracy of the model. In this work we propose to study this phenomenon by means of a spatially projected eigenvector centrality function. Albeit simple, we show that this technique is computationally efficient and has the potential for predicting transport phenomena in porous media. The porous medium is viewed as a pore-network where the pores are associated to nodes, and pore throats to edges connecting pores. We propose a method to compute the spatially projected eigenvector centrality (SPEC) to perform a topological characterization of the pore-network. We implement a correction of the common eigenvector centrality measure to overcome a centralization problem, and a method to bias the centrality distribution along a particular direction is introduced to address the flow and transport anisotropy in porous media. Direct comparison with experiments shows that this proposed SPEC function allows to predict the preferential paths and stagnation zones for flow and transport in the porous medium. Moreover, we show that the entropy and connectivity as computed from eigenvector centrality allows for a further characterization of the network.

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Generalized modelling and experimental validation of stagnant thermal conductivity of porous materials

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The effective thermal conductivity is a parameter commonly used to characterize the overall thermal behavior of multi-phase systems according to a homogeneous approach. Generic models describing the effective thermal conductivity of porous materials, such as sponges (open-cell metal foams), rely on parameters fitted to experimental data. These parameters may depend on structural properties, the manufacturing process, and single phase thermal properties of the porous material. On the other hand, a derivation of the effective thermal conductivity by means of numerical calculations (Finite Volume Method, FVM) requires the use of computer tomography (CT) scans of the material or at least the generation of similar geometric structures, such as Wheire-Phealan structures. A combined experimental and numerical approach for deriving the fitting parameters of generic models for classes of porous material is proposed to combine the advantages and to overcome the respective drawbacks of each single method.

One example for a generic approach is the model proposed by Krischer [1], which is based on an Ohmic combination of serial and parallel thermal resistances. An adaption of the Krischer model, depicted in Figure 1 (left), is suitable for describing the effective conductivity of some ceramic sponges [2]. The weighting parameter, b, accounts for the proportion of serial and parallel conduction and can be derived experimentally or numerically. Using literature data, it was determined that this parameter must be adapted for each specific class of materials. To derive this dependency in a general way, the structural and thermal properties are described by a more complex network of thermal resistances. The strut thickness, strut length and thermal conductivity of the bulk material may be taken into account by this approach. Easy algebraic calculations can then be used to determine the overall thermal resistance of the material which, in turn, allows for the estimation of the form parameter b. Figure 1 depicts the level of sophistication of the different approaches.

To validate the proposed procedure, the weighing parameter, determined by analyzing the resistance network for different classes of porous materials, is compared to both experimental and numerical data. A guarded hot plate test facility has been designed to measure the effective conductivity of small, highly conducting samples precisely. Thermal conductivities of both regular and irregular porous metals and ceramics are presented and compared to literature data. FVM calculations rely on the CT scanning of ceramic sponges with a porosity of approximately 90 % and a variation of the bulk material thermal conductivity for irregular structures. In the future, the resistance network analysis is to be expanded to derive a general, simple model for describing the effective thermal conductivity of different classes of multi-phase materials.

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Generalized multiscale discontinuous Galerkin method for solving the heat conduction problem with phase change

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In this work, we consider the numerical solution of heat conduction problem with phase change in perforated domains. For the simulation of heat transfer processes with phase transitions the classic Stefan model is used.

Computational implementation is based use of generalized multiscale discontinuous Galerkin method (GMsDGM). Considered method GMsDGM is based on the interior penalty discontinuous Galerkin method as the coarse grid solver. In contrast to Generalized Multiscale Finite Element Method (GMsFEM) which uses continuous Galerkin methods. The main idea these methods is to construct a small dimensional local solution space that can be used to efficient solution on coarse grid.

We present numerical results for geometry with a lot of perforations to demonstrate the performance of our method. Results of numerical simulation problem in perforated domains in two-dimensional and three-dimensional formulations are presented.

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Hybrid MultiScale Finite Element-Finite Volume Framework for the Coupled Biot's Equations

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Geological porous media display highly heterogeneous hydromechanical properties over a wide range of length scales that require high resolution characterizations to obtain reliable modeling predictions. Multiscale-based strategies offer a natural solution route to tackling the computational burden. We propose a novel hybrid MultiScale Finite Element-Finite Volume framework (h-Minisymposium FE-FV) for the simulation of single-phase flow through a deformable porous medium based on Biot's poromechanics theory. A two-field fine-scale mixed finite element-finite volume formulation, which assumes the displacement vector and pressure as primary unknowns, is first implemented for the system of coupled balance equations for linear momentum and mass. For the Minisymposium FE displacement stage, we introduce local basis functions for the displacement field over coarse elements that are subject to reduced boundary condition. Such Minisymposium FE stage is then coupled with the Minisymposium FV method for flow, in which a coarse and a dual-coarse grid are imposed to obtain approximate but conservative multiscale solutions. Robustness and accuracy of the proposed method---both as an approximate, non-iterative solver, and a preconditioner---are demonstrated by several numerical examples.

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Multiscale Model for Compositional Transport

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A coupled description of flow and the compositional changes is spanning a wide range of length and timescales. Adding to the complexity is the subsurface heterogeneity with complex multi-scale features. Hence we need appropriate and suitable methods that are robust to solve these interactions at the subsurface. A compositional model is a reliable option for understanding of complex subsurface processes with strong changes in initial composition and corresponding multiphase interactions. It is usually applied for the simulation of Enhanced Oil recovery (EOR) processes, specifically for the gas injection where one needs to determine an optimum injection composition of gas for achieving the maximum oil recovery. In this type of simulations, the oil and the gas composition are described as a mixture of nc individual components where each component is associated with the corresponding mass balance equation. In addition, we need to perform the phase stability test and the flash calculations to estimate the distribution of components between phases which ultimately increases the complexity of the simulation and thereby the simulation time. A compositional space parameterization approach [1] is used to improve the performance of compositional simulation which is based on the parameterization of a compositional solution related to the thermodynamic phase behavior of the system. The problem is solved based on the tie line variables and phase fractions. It was also observed that projection of the full compositional solution in the tie line space is invariant with respect to hydrodynamic properties [2]. Here we utilize this technique to develop a fine scale reconstruction based on a coarse scale solution where nc governing equations at fine scale are effectively reduced to two. This helps us to drastically reduce the simulation cost of compositional simulation without significant loses in accuracy.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 842

Double-porosity hydro-mechanical model with application to analysis of bentonite based sealing elements

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We consider a Biot type hydro-mechanical model combining flow in variably saturated porous media described by the Richards equation and deformation of the porous matrix. In the case of bentonite based sealing structures, the deformation is caused by swelling and interaction of the sealing structure with the environment (the host rock). In the presence of the initial voids, the deformation and the corresponding change of the pore space can be large and such deformation influence the flow parameters as saturated permeability and the water retention function. Then a model of the water retention function as a relation among saturation, suction and deformation (dry density) has to be used. In this contribution, we describe a construction of such water retention function and its incorporation into Richards equation. This construction takes into account a double porosity structure of the bentonite with micropores and macropores, where only the macropores are significantly influenced by deformation. We also show the application of the developed model to analysis of one of the SEALEX experiments, which were realized by IRSN in Tournemire underground rock laboratory in France. This analysis was performed within the DECOVALEX 2015 project; see e.g. Millard et al., Comparative modelling approaches of hydro-mechanical processes in sealing experiments at the Tournemire URL. Environ Earth Sci (in review). Additionally, this modelling involves a specific approach for modelling the initial void between the sealing structure and the host rock as well as modelling the gaps between bentonite blocks.

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Integrity Analysis of Sealing Components of the Engineered Barrier System in a Repository for Heat-Generating Radioactive Waste and Spent Fuel based on Thermo-Hydro-Mechanical Simulations

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In the Federal Republic of Germany, the final disposal of heat-generating radioactive waste and spent fuel in clay formation is investigated as an alternative to the concept in salt formation. Clay is characterized by a very low permeability which makes it suitable for industrial sealing applications. On the other hand, Clay provides a high retention for radionuclides due to its sorption capabilities. For these reasons, clay is qualified as geological formation for the disposal of radioactive waste. The isolation of radioactive waste in deep geological formations is provided by a multi-barrier system based on a combination of engineered and natural barriers. The natural barrier is provided by clay itself whereas the engineered barrier is made of geotechnical sealing components installed at specific locations in the excavated repository. For the long-term safety of a repository in clay formation, the integrity of the natural barrier has to be proven for a time period of 1 million years. The structural integrity of the geotechnical sealing components has to be proven for the transient phase characterized by repository induced changes. The goal of this study is to determine the loads acting on the sealing components in order to perform the integrity proof of the elements of the sealing system. For this purpose, thermo-hydro-mechanical effects which occur in the near field of the repository were simulated numerically. Two numerical models have been developed to simulate the loads acting on the drift seals and the borehole seals. Obviously, due to the saturation of the backfill and the seals, the increasing pore pressure and the thermal expansion of the porewater, the rock and the sealing elements themselves are the principal loads acting on the sealing elements. Based on the calculated loads and the resulting deformations, the structural integrity can be analysed and the integrity proof be performed. The integrity proof is based on five criteria which have to be met by the engineered barrier: the structural stability, the crack limitation, the deformation limitation, the filter stability and the durability criterion. Preliminary results show that the integrity of the borehole seal can be proven. The simulations of the drift seal model are still in progress.

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Modeling Damage and Fluid Flow in the EDZ using the Discrete Element Method

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Local stress changes caused by drift excavation in a deep geological repository in rock salt lead to the evolution of an excavation damaged zone (EDZ) adjacent to man-made openings. The EDZ is a region where progressive failure occurs. This decreases the material strength and increases the permeability of the originally tight host rock. In general, such an EDZ can have a major impact on the long-term safety of a radioactive waste repository since it can violate the integral sealing function of geotechnical barriers. It is known that the microstructural damage is due to the initiation and propagation of microcracks. With increasing damage, the coalescence of individual fractures results in a pervasive fracture network where a sudden increase in permeability can be observed. However, many methods used to simulate the mechanical and hydraulic processes inside the EDZ are based on continuum mechanical approaches where the microcracks can only be investigated to a limited extent. The objective of this study is the development of a modeling strategy that can be used both to simulate the damage of rock salt at the grain scale and to determine the fluid flow of fracture systems simulated. For this purpose, discrete element modeling techniques were used in combination with polyhedral shaped elements (Voronoi polyhedra) in order to duplicate shape and arrangement of grains. To calibrate the mechanical material parameters used in the constitutive models and to validate the relevant damage and fracture processes, uniaxial compression tests were combined with acoustic emission measurements in a first step. The simulated stress-strain relationships showed good agreement with laboratory results. Moreover, a good agreement was achieved in respect to spatial and temporal occurrence of fractures. The next step involves the generation of realistic fracture networks occurring in the EDZ using the DEM approach. The excavation of a drift is first simulated with continuum mechanical approaches to determine the in situ stresses that occur in the region surrounding an excavation. The stresses are then transmitted as boundary conditions onto a DEM model to simulate the fracturing for different depths in the EDZ at grain scale. It was shown that the resulting damage in the discrete model is anisotropic. This is in agreement with observations where the fractures of the EDZ are principally orientated parallel to the direction of the maximum principle stress. As a final step, the fluid flow in the fracture systems generated was quantified by calculating the three dimensional hydraulic conductivity tensor. This allows the specification of directionally dependent (anisotropic) permeability properties that can be used as input parameters for continuum models simulating the fluid flow at larger scales.

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Non-destructive tomographic monitoring of transport processes in barrier material (Opalinus clay) with PET

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Parameterizing transport in barrier materials is a challenge, because the processes are extremely slow, limited to smallest quantities, and frequently strongly localized, e.g. to fractures. These processes are generally well characterized on the molecular scale, but strongly affected by structural effects on the larger scales. Due to the intricate derivation of experimentally substantiated parameters, the impact of these scaling effects is often unduly neglected in process simulations for safety assessment. As most sensitive tomographical modality, which is capable to monitor traces with molecular concentrations on macroscopic samples, we apply positron-emission-tomography (PET) with a high-resolution scanner („GeoPET“) for parameterizing transport in barrier materials (Kulenkampff et al. 2016a). We focus here on diffusion in Opalinus clay as potential barrier rock for nuclear waste deposits (Kulenkampff et al. 2016b, 2016c). Our method is complementary to diffusion experiments in small diffusion cells and additionally provides information on heterogeneity and anisotropy of the process. We derived anisotropic diffusion coefficients from the measured spatiotemporal tracer distribution which are in accordance with results from diffusion cells (Lippmann-Pipke et al., 2016). The spatial characteristic of the tracer distribution suggests that this anisotropy is caused by preferential transport along fine layers on the millimetre to centimetre scale. This finding should be considered in process simulations, because it means a reduction of the volume that effectively is affected by the process and thus faster progress of the tracer and a reduction of the reactive internal surface area, when adsorption is considered. Other examples, where we take advantage from the favourable features of the GeoPET-method, are advective fluid transport in fractured salt and crystalline rocks, as well as reactive injection of water glass into salt rock. In all these cases we monitor tracer concentrations and thus the key parameter for reactive transport modelling. We recommend GeoPET as unique experimental method to verify transport simulations on the macroscopic scale of drill cores.

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oops! Open Object-Oriented Parallel Solutions: A C++ Class Library for the Solution of Transport Equations

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Geothermal energy utilization is the main area were we use numerical models to develop and enhance process understanding and to predict the dynamics of the system under consideration. Other topics include sponta- neous underground coal

res and subrosion processes. Although the details make it inconvenient if not impossible to apply a single code implementation to all systems, their investigations go in similar ways. They all depend on the solution of coupled transport equations. We thus see a need for modular code systems with open access for the various communities to maximize the shared synergistic e
ects. To this purpose we develop the oops! (open object-oriented parallel solutions) - toolkit, a C++ class library for the numerical solution of mathemati- cal models of coupled thermal, hydraulic and chemical processes. This is used to develop problem-speci

c libraries like acme(amendable coal-

re modeling exercise), a class library for the numerical simulation of coal-

res and applications like kobra (Kohlebrand, german for coal-

re), a numer- ical simulation code for standard coal-

re models. The latest development just started is the SIMBA toolkit for the simulation of geothermal plants. Basic principle of the code system is the provision of data types for the description of space and time dependent data

elds, description of terms of partial di
erential equations (pde), their discretisation and solving meth- ods. Coupling of di
erent processes, described by their particular pde is modeled by an automatic timescale-ordered operator-splitting technique. If in a derived speci

c application library functionalities of general interest are implemented and have been tested they will be assimilated into the main library. Interfaces to external pre- and post-processing tools are easily im- plemented. Thus a construction kit which can be arbitrarily amended is formed.

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Thermo-hydro-mechanical behaviour simulations in Boom Clay for a radioactive waste repository

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In the Netherlands, radioactive waste is proposed to be disposed in a repository situated in the Boom Clay layer at approximately 500m depth, following 100 years of above ground storage. Boom Clay is a plastic clay which is highly impermeable. An initial assessment of the thermo-hydro-mechanical behaviour is presented here. The temperature rise is significantly lower than in other proposed programmes due to the long period of above ground storage, although this is accompanied by a significant rise in pore pressure, calculated to be in the region of 1-2MPa. It is shown that, by using mid-range material parameters this causes a reduction in the plastic zone between disposal galleries (see Figure 1). However, the behaviour is highly sensitive to the thermal expansion coefficient of the Boom Clay, which in itself is not well known (and is non-linear). By considering an increase of the coefficient of thermal expansion, within stated values in literature, the plastic zone can be seen to increase substantially, becoming continuous between the disposal galleries (see Figure 2). This has the potential to increase the loads on the tunnel linings and to create a large disturbed zone, which should be then considered in the safety assessment.

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A Full 3D Mixed Hybrid Finite Element Model of Superabsorbent Polymers

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Superabsorbent polymers (SAPs) are cross-linked polymer networks with large negatively charged ion groups attached to the solid matrix (polymer chains). By the presence of these large negatively charged ion groups, osmotic pressure difference rises in and outside of the gel. The osmotic pressure difference is, as a matter of fact, the main cause for the exceptional swelling ability of SAPs. In this study, we present a dynamic Mixed Hybrid Finite Element (MHFE) model in three dimensional setting for the simulation of the finite swelling of SAPs (Figure 1). In the model, the normal flux is approximated using Raviart-Thomas elements, which conserve mass both locally and globally. The solid part is assumed to be isotropic and hyperelastic under isothermal conditions. The transient simulation results are verified with a semi-analytical solution in one dimension (Figure 2); while the 3D equilibrium results in the case of a spherical geometry are verified against the analytical solutions. As a result of good agreements between the simulation results and analytical solutions, the mixed hybrid finite element method is demonstrated to be a robust and accurate numerical method for 3D simulation of a volume increase of even more than 2500%. Moreover, we take into account the heterogeneity in permeability exhibited by the hydrogel during swelling. Specifically, the outer part of the gel shows much higher permeability than the core due to the increased size of the pores. We are able to prove the computational superiority of the mixed hybrid method over the conventional finite element method in terms of accuracy and computational efficiency when they are applied to this type of model problem.

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A robust numerical scheme for two-phase flow in porous media

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In this work we present a mass conservative numerical scheme for two-phase flow in porous media. A global/complementary pressure formulation is considered. The proposed numerical scheme is based on backward Euler for the temporal discretization and mixed finite element method (MFEM) for the spatial one. A Hoelder continuous saturation, not necessary strictly increasing is considered. The convergence of the scheme is rigorously proved. The convergence rate is naturally depending on the Hoelder exponent. The non-linear systems within each time step are solved by a robust linearization method, called the L-method. This iterative method does not involve any regularization step, and the linear solvers within each iteration are much better conditioned as in the case of Newton's or Picard's method [1]. The convergence of the L-scheme is rigorously proved under the assumption of a Lipschitz continuous saturation [2,3]. For the Hoelder continuous case, a numerical convergence is established. Illustrative numerical results are presented to sustain the theoretical findings.

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AD-GPRS: Flexible and Efficient Multiphysics Multiscale Research Platform

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We present a platform for simulation of complex coupled multi-physics processes. The simulator has a modular design with modules representing, e.g., compositional flow, energy transfer, mechanical deformation, chemical reactions, wells, or electrical current. The platform provides flexible and efficient coupling between the modules and enables different solution strategies from a fully coupled approach to all possible sequential schemes. Each module has a choice of nonlinear formulation, discretization method, nonlinear and linear solvers. We discuss the design of the framework and demonstrate applications for a variety of challenging geoengineering problems including steam assisted gravity drainage, cold water injection, acid injection, in-situ upgrading, geothermal energy extraction. Besides that, we also show the possibility to investigate the robustness and computational efficiency of different coupling strategies for a given problem. We demonstrate that the framework provides options not only for coupling of different physics but also allows operating with different subdomains and scales of description.

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Coupled water and energy transfers in porous media with freeze/thaw: permaFoam, a massively parallel OpenFOAM® solver

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This work presents a numerical solver for the multiphysics problem of hydric and thermal transfers in variably water saturated porous media with freeze/thaw of the poral water. The application that we aim to deal with is the study of the dynamics of permafrosts, which are constituted of soils and geological bodies frozen in depth all year round, with a thawed superficial active layer in summer. Permafrosts are present on about 20 % of continental surfaces, i.e. ~25 millions of km². The mid term objective of this numerical development effort is to contribute to the quantification of the impacts of climate change on the weathering fluxes from the boreal areas to the oceans (e.g. : [1]), although other potential fields of application exist (e.g.: engineering in cold regions). This kind of cryohydrogeological problems involves strong couplings and strong non-linearities, and the development of related numerical solving tools has been the subject of a renewed interest during these last years (e.g.: [2]). Here we present the cryohydrogeological solver permaFoam [3] which has been developed in the framework of the open source tool box for computational fluid dynamics OpenFOAM®. PermaFoam allows the coupled resolution of a modified Richards equation that takes into account the decrease of hydraulic conductivity related with the freezing of the pore water and of an advection-conduction equation which includes a latent heat exchange term. The use of OpenFOAM® allows to benefit from its excellent parallel performances (e.g.: [4]). This latter point is crucial given that the strong non linearities and the steep fronts encountered in cryohydrogeological modelling may induce very important computation times. After a short introduction of the considered equations and of the used numerical methods, some analytical validations and code-to-code comparisons performed in the framework of the international benchmark Interfrost [2] will be presented. The parallel performances of permaFoam will then be discussed on the basis of strong scaling curves obtained with the supercomputer EOS (CALMIP High Performance Computing center). Finally, the capabilities of permaFoam will be illustrated with an example of application in a monitored catchment of Central Siberia, the Kulingdakan watershed (e.g.: [5], [6]).

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Grid generation for large scale simulations of density driven flow on highly anisotropic layered domains

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Simulations of realistic physical problems require detailed virtual representations of the underlying physical domains. The construction of such domains can be a challenging task, since not only the shape but also the structure of the generated nets play an important role in the efficiency of the applied discretization and solving techniques.

We describe several interweaved meshing techniques to generate prism based, semi-unstructured, anisotropic coarse grids, recovering inner and outer layer boundaries using our meshing software ProMesh. On the fly, we generate projectors which allow to construct non-nested multigrid hierarchies through repeated refinement. The refined mesh thereby resembles the original domain better with each refinement step.

Employing the parallel capabilities of our simulation software UG, those hierarchies can be constructed in parallel to allow for massively parallel simulations of density driven flow on layered domains. We present results of such simulations and discuss efficiency and convergence of the employed solvers.

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High-order hybrid discontinuous galerkin methods for diffusion-convection equations with evanescent diffusion

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Recently, connections between the hybridization technique and mixed discontin- uous Galerkin (MdG) methods have been successfully explored to derive a new family of Galerkin finite element methods. The hybrid discontinuous galerkin (HDG) methods was introduced in [4] and accuracy was proved to be better than MdG methods and represent a very competitive alternative to the well-known mixed-hybrid H(div)-conforming methods using either Raviart–Thomas (RT) or Brezzi–Douglas–Marini (BDM) families (see [1]) in purely elliptic cases. Here we focus on convection dominated cases and analyse the effects of a lo- cated diffusion vanishing. Using the HDG approach in the well-known diffusion- convection equation, we try to describe purely discontinuous phenomenons through the evanescent diffusion case. To do this, we introduce a so-called alpha-method in the weak formulation to consider a null diffusivity term in part of a domain where only convective transfers will occur. To get a global approximation of the flux describe into porous medium, we have chosen to include diffusion and convection flux together such that the conservative law will consider the both phenomenons with their own flux base approximations. The stabilisation parameter τe in the conservative equation is taken in accordance with the upwinded scheme. A comparative study is made between the two versions of the stabilisation term introduced in [4] and [3] to present the efficiency of the two schemes in terms of computational time and accuracy. A local postprocessing introduced in [5] and [2] is implemented to improve the superconvergence of the HDG scheme and to apply H(div)-conforming proper- ties in the flux estimate which is verified on RT and BDM elements. Finally, the numerical results are presented in a table which link element and hp refinement procedures together to describe their convergence properties. For more graphical examples, the errors of the different schemes are plotted in the same graph to highlight their particularities. Comparison with RT -hybridized elements is made and we conclude about the outlook carried out by the scheme presented in approximations of discontinuous solutions in porous medium.

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Numerical Model for Three-Phase Flow in Poroelastic Media

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A new computational model is developed for solving three phase compressible flow in heterogeneous poroelastic media. The model begins by addressing the fully-coupled formulation, processed within the context of the fixed stress split algorithm [1,2] wherein the Lagrangian porosity is computed using the constitutive law proposed by Coussy [5] and the volumetric strain eliminated from the effective stress principle [3]. Such procedure gives rise to a new iterative formulation wherein the original fully-coupled model is decomposed into three subsystems associated with the hydrodynamics, geomechanics and the set of conservation laws for the saturations of the liquid phases. The hydrodynamics is governed by a new form of the pressure equation with an additional source term arising from the evolution of the total stress premultiplied by saturations and formation volume factors of the fluid phases. The new pressure equation is written in conservative form with nonlinearities treated by a Newton-type scheme whereas the nonlinear coupling between flow and transport is handled by a proper sequential iterative scheme. The predictor step is discretized by a higher order finite volume method whereas the corrector captures the influence of the geomechanics upon transport quantified by the source term in the system of hyperbolic equations [4]. Numerical results illustrate the influence of geomechanics in the oil production curves in WAG (water alternate gas) scenarios.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 946

On the application of CFD for establishing a protocol for Representative Elementary Volume (REV) definition in pore-scale modeling of reservoir rock

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Flow and transport in porous media is vital to many areas of engineering and science, including groundwater hydrology, subsurface CO2 sequestration, and Hydrocarbon production from underground reservoirs. Image-based pore-scale modeling of transport phenomena has become an important tool for understanding the complicated relationships between the pore structure and the measurable macroscopic properties; in particular, the effective permeability. The main venues for pore-scale modeling are network extraction and the Computational Fluid Dynamics (CFD). The latter CFD approach has been rendered successful in handling cases with large heterogeneity, and attempts to solve the Navier-Stokes equations on the complex boundary conditions of the inner-rock pore spaces. The present work uses the OpenFOAM software to determine the effective permeability of (Bentheimer) sandstone rock. Our methodology was based on extraction of stereolithography (STL) surfaces from the CT-scan images of reservoir rock, which was implemented by our in-house developed computer code. The code is capable of preserving the precision of surface extraction by as low as the resolution of the CT-scan images (4 micrometers). Simulation of fluid flow within the STL surfaces was later attempted by OpenFOAM. To explore the effect of image subscaling on effective permeability, different subsets of the entire micro-structure domain were used for CFD simulation. The results indicate that variation in effective permeability of subset rock samples decreases by increasing the size of the pore-scale sample and favorably converges to the value established for the entire domain, as the size approaches 250x250x250 (voxels). Similar results were obtained as for the porosity of subset pore-scale samples. The results are invaluable in establishing an authentic protocol for definition of Representative Elementary Volume (REV) within the CFD pore-scale modeling context.

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Parallel and adaptive finite volume simulations for density driven flow

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Present-day supercomputers with hundred thousands of cores provide an enormous computing power and large-scale simulations for flow in porous media can benefit from these resources allowing refined and more detailed simulations. Using grid-based finite volume discretization methods, we solve the governing equations of porous media flow using multigrid methods on massively parallel architectures. We present the employed parallelization strategy and its implementation together with empirical scaling results. In addition, the aspect of grid-adaptivity for the employed finite-volume scheme is considered.

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Particle migration in porous media simulated combining Lattice Boltzmann, Immersed Boundary, and Discrete Element Methods

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During water flooding of oil reservoirs, fine particles (or fines) are produced by erosion or chemical weathering, especially in sandstone formations. The fines can then migrate with the fluid and either blocking or decreasing the cross section of the pore throats by bridging and deposition[1]. On one hand, negative consequences are the reduction of conductivity and damage of formation. On the other hand, sweep efficiency and oil recovery might improve[2]. It is therefore of great importance to understand the migration of fines during water flooding in order to protect the formation and improve the production. Several earlier works on this issue have focused on numerical simulations of fines. E.g., Foppen and Schijven[3] built the solute transport mass balance equations to simulate fines transport and optimized their calculations on laboratory experiments, determining model parameters. Bedrikovetsky et al.[4] proposed a new mathematical model for the detachment of particles based on mechanical equilibrium which can calculate the maximum retention concentration and formation damage coefficient. Finally, Yuan and Shapiro[5] used a reservoir model designed for polymer flooding to simulate fines-assisted water flooding. All these modeling approaches are able to predict the blocking forms and the permeability variation of the reservoir. However, they cannot describe the particle motion in the porous media directly and neglect the discontinuous characteristic of particles in two-phase flow.

In this paper, we developed a direct numerical simulation (DNS) method to simulate the fluid-solid two-phase flow in porous media. First, we implemented the hydrodynamic model of fluid flow based on the lattice Boltzmann Bhatnagar–Gross–Krook (BGK) model with the force term, which has been proved to be a useful tool for simulating complex fluid flows and transport phenomena. Second, we described the fluid-solid interaction by a momentum exchange-based Immersed Boundary Method[6]. In the mesh generation, the fluid domain was covered by Eulerian square lattices and the particle boundary was represented by a set of Lagrangian points. Finally, the particle motion was evaluated by the Discrete Element Method, where the active forces between particles are divided into five components: buoyancy, gravity, collision force between particles, interaction of particle and fluid, collision force between the particle and the rock. We therefore used the developed couple model to study fines migration problems in porous media and gain an insight into the effects of particles on the change of fluid velocity, permeability, and sweep coefficient. An example of simulation results to show the effect of fines to velocity vectors in the field and velocities in the outlet compared with the non-fines condition are shown in Figure 1 and 2 separately.

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Phase-field modeling of fracture in partially saturated porous media

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Porous media such as soil, rocks and concrete are of great importance in the context of civil engineering and environmental geomechanics. They consist of a solid skeleton and pores filled with fluids, e.g. air and water. Complex mechanisms of flow and transport take place within the pore network and can lead to deformation of the solid skeleton and eventually to fracture phenomena. Phase-field modeling of fracture has recently emerged as an alternative to conventional approaches such as remeshing, extended finite element methods or cohesive zone modeling. The phase-field framework can be considered a special type of gradient damage modeling approach, where a diffusive approximation of the crack is taken into account and the continuous phase-field parameter is used to describe the material integrity. The essential advantages are the possibility to describe arbitrarily complicated fracture patterns such as nucleation, branching and merging, without ad-hoc criteria on a fixed mesh, through the solution of partial differential equations derived from variational principles [1, 2, 3, 4]. Phase-field modeling of fracture in porous media has been addressed in some recent publications [5, 6], which however have only focused on the fully saturated case. Objective of this contribution is to describe fracture in partially saturated porous media using a phase-field approach. In this study, the material is described by its linear-elastic properties. The overall balance of linear momentum, the continuity equation and the phase-field evolution equation constitute a nonlinear coupled and time-dependent system of equations, which needs to be discretized and linearized. We formulate the coupled non-linear system of partial differential equations governing the problem with displacements, capillary pressure and crack phase-field as unknowns. The spatial discretization is carried out with finite elements of appropriate order for the different unknowns. We discuss its solution and present some relevant examples.

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ReactMiCP : a modular reactive transport simulator for variable-porosity problems

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Supplementary cementitious materials such as fly-ash or blast-furnace slag, are added to cement to reduce the carbone footprint of concrete. However, to guarantee the long-term durability of the concrete made from these new formulations, we need to understand the effect of these additions on the chemical and mechanical properties of the binders. In particular, our models need to capture the long-term degradation mechanisms and how they relate to the evolution of the microstructure. Inside a porous medium, the different phenomena are coupled by the microstructure and its evolution. For example, in coupled simulation of drying and carbonation, the entry of CO2 and release of water will occur through the carbonated layer which has distinct properties from the non-carbonated core.

We propose a new reactive transport simulator for variable porosity problems. The implementation was developed to expose an application programming interface so modelers can develop task-specific simulators. In particular, they can integrate a custom-made microstructure model adapted to the problem at hand. Using it, we can follow the evolution of the microstructure as function of the advancement of the chemical reactions in complex porous materials. We demonstrate the abilities of our simulator using two systems. The leaching of cement paste in contact with acid brines and a coupled simulation of drying and carbonation of cement paste. In both cases, our numerical abilities exceed the experimental data available. New studies combining advanced simulations tools and new experimental tools are needed to achieve quantitative prediction abilities.

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Simulation of multi-physics materials in commerical softwares

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From a micro-structural point of view, many natural or engineered materials can be assigned to the class of multi-physics materials. Therein, their macroscopic observed behaviour is governed by different micro-structural physical phenomena. For instance, when electro-active polymers (EAP) are subjected to a electric field, the resulting chemical and electrical imbalances trigger micro-structural diffusion processes, which re-establish the equilibrium state, thereby causing macroscopic deformations. Further examples for these materials are partially or fully saturated porous media (e. g. foams, soils, filters, fibre-reinforced plastics), chemical- or electrical-active materials (e. g. hydrogels, lithium-ion batteries) or biological tissues (e. g. bone, cartilage). Addressing the simulation of multi-physics materials, which often exhibit a complex and heterogeneous micro-structure, it is convenient to proceed from a macroscopic modelling approach. In this regard, the aforementioned materials can be described exploiting the macroscopic Theory of Porous Media (TPM), see [1], as a suitable modelling framework.

Addressing the simulation of multi-physics materials, the present contribution bridges the cap between research and industrial application. In particular, the governing material model, which are usually developed during either academic or industrial research projects, are often implemented into dedicated software packages or programme codes to elaborate its advancements and its limitations. In contrast, within the industrial application, a stable software and a user-friendly software package is required, thereby allowing for the definition of complex initial-boundary-value problems (IBVP), which is a requirement research codes usually do not comply. To cope with this, the present contribution addresses a general interface between the research code PANDAS, which is a multi-field finite-element solver, and the commercial finite-element (FE) packages Abaqus, see [3], and LS-DYNA. The coupling is based on the user-defined element subroutines of Abaqus and LS-DYNA, respectively. This procedure allows, on the one hand, a straight-forward embedding of all material models of PANDAS into commercial FE packages. On the other hand, it provides, in comparison to the native user-defined subroutines, a user-friendly programming environment for user-defined material models with an arbitrary number of degrees of freedom. Furthermore, the coupling exhibits minimal-invasive properties with respect to the IBVP definition process and allows for the parallel analysis of large-scale problems on high-performance computing clusters. The capabilities of the coupling procedures are illustrated by the simulation of various coupled multi-field problems, such as partially or fully saturated soils, vacuum-assisted resin injections (VARI) of dry fibre fabrics, see [3], or chemically or electro-chemically driven swelling phenomena as they appear, for example, within hydrogels [2].

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Smoothed Particle Hydrodynamics model of poroelastic media

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We investigate hydraulic fracturing including fracture propagation in porous media. As a first step, we numerically investigate an implementation of a biphasic poroelastic medium assuming incompressible solid grains and negligible effective pore fluid density and a linear-elastic constitutive equation for the extra stresses of the solid phase [1]. Generally, classical numerical methods such as X-FEM are employed to solve similar poroelasticity problems [2]. However, the pre-processing and remeshing steps involved in mesh-based methods are highly computationally expensive. To overcome this shortcoming, we solve the governing balance equations applying the Smoothed Particle Hydrodynamics (SPH) [3]. SPH is a mesh-less Lagrangian method highly suitable for large deformations [4]. The model is proposed for solving problems in the framework of geothermal explorations, requiring to simulate large domains that may be representative for the reservoir scale. Therefore, we implement the SPH solution in a parallel computational framework. For validation of the proposed model of poroelasticity we numerically investigate some classical consolidation problems and a 2d borehole case. Furthermore, we compare the pressure diffusion results with analytical solutions.

In addition, we extend the SPH poroelastic approach to model fracture initiation and evolution in porous media, simulating fractures as a smeared scalar field with a hybrid approach based on coupled SPH and Phase Field methods [5]. With the proposed method, we overcome the instabilities that can occur in the SPH method when fracture initiation occurs. The first validation of the proposed hybrid model is made in single phase solids. The model is afterwards enhanced to model fractures in porous media.

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Swelling driven crack propagation in large deformation in porous media

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Ionized soft porous media, such as hydrogels, soft tissues, are considered as a saturated two-phase mixture, consist of a charged deformable solid skeleton and an interstitial fluid of opposite charge. In biomedical engineering, hydrogel is a common physical model for soft tissues and consists of cross-linked ionized polymers. The equilibrium swelling behavior of a cross-linked gel is well know [1, 2]. The focus also goes to the kinetics of swelling during bending and twisting, as well as geometry impact and the dynamics of deformation by non-homogenous swelling [5]. Fewer studies take defects of the hydrogel into consideration. Hydrogels subjected to changes of salt concentrations often develop cracks during swelling or shrinking [4]. In return, the presence of discontinuities influences the swelling mechanics of the porous media, like swelling capacity. Therefore, it is strongly desirable to study the coupling between the fluid pressure and crack propagation.

In this paper, we present a swelling driven fracture model for porous media in large deformation. Flow of fluid within the crack, within the medium and between the crack and the medium are accounted for. The partition of unity method is used to describe the displacement field and chemical potential field respectively. In order to capture the chemical potential gradient between the gel and the crack, an enhanced local pressure model is applied[3]. The capacity of this numerical model to study the fracture and swelling behaviors of gels with low Young's modulus and low permeability is determined. We present a numerical example to show the performance of the current model. Figure 1 is the geometry and boundary conditions of swelling driven fracture test. A changing chemical potential is applied along the surface (blue solid line), the horizontal red solid line indicates the initial crack (R = 0.5 mm). Figure 2 and 3 are the chemical potential distribution in the gel and in the crack respectively. From the simulation , we demonstrate the capacity of ELP model in reproducing crack propagation in large deformation with low Young?s modulus (O(MPa)) and low permeability (O(10-4 mm^4/Ns)).

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The dumux- multidimension module for coupled problems in porous media

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There are many engineering applications for porous media where two or more systems with different dimensions are coupled such as blood-flow in capillaries with the surrounding tissue, pore-network models coupled to a Darcy or a free-flow domain, fracture modeling or root water uptake with a root architecture as the one-dimensional domain embedded in the three-dimensional soil domain. Dumux-multidimension, a sub-module of the open-source numerical simulator DuMuX (Flemisch et al. 2011) offers the infrastructure for the coupling of various models on different scales. Here, one sub-problem is defined on a bulk domain and the other sub-problem is defined on a lower-dimensional domain. The lower-dimensional problem might live on the bulk grid's facets (codim 1 entities), touch the bulk domain on its boundary, or be arbitrarily embedded into the bulk domain. The domains are represented discretely by two independent DUNE grids which offers the possibility to couple complex geometries. Dumux-multidimension uses dune-foamgrid for the lower-dimensional problem which is a recent DUNE grid interface implementation for one- and two-dimensional grids in a physical space of arbitrary dimension. (Sander et al. 2015) The coupled problem can be solved in a fully-implicit manner, resulting in a monolithic system matrix, or iteratively, yielding two individual linear systems of equations which gives the possibility to use different time discretizations and different solvers for the sub-problems. Switching between those two solution strategies can be achieved at runtime allowing for fast and simple comparison between schemes. A coupling class, implemented for a new problem type, manages transferring user data from one sub-problem to another. The sub-problems itself are regular DuMuX problem classes that require only minor invasive changes to obtain an algorithmically strong coupling. Thus, great flexibility in terms of coupling mechanisms is retained and all models available in DuMuX can be employed as sub-problems in a coupled problem.

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Validity of models of density-driven flows in porous media with low-dimensional fractures

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Fractures are typical components of hydrogeological media. As they introduce strong heterogeneities, their influence on the flow of the liquid phase is essential. Due to their small aperture, they are often considered as low-dimensional object. This allows to avoid difficulties with numerical methods in the simulations. Although this simplification provides a good accuracy for potential flows, it results in neglecting important phenomena in the density-driven case. This leads sometimes to wrong simulation results that cannot be recognized in the context of the simplified model itself. In the talk, we investigate the restrictions of the validity of the models of the density-driven flows in porous media with the low-dimensional representation of the fractures. For this, we consider the role of the vorticity of the flow field inside the fractures. We propose a criterion for the validity and verify it by numerical tests. Furthermore, we construct and test a dimensionality-adaptive technique for the simulations of this type of the flows.

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Diffusion in clays. Continuum and micro-continuum approaches

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The mineralogical and chemical properties of clays have been the subject of longstanding study for several important subsurface energy-related applications, including the long-term disposal of nuclear wastes in geological repositories and the storage of CO2 in subsurface geological formations. In these applications and environments, the low permeability of clay materials provides at least part of the safety functions for radionuclide contaminants confinement and subsurface CO2 sequestration. From a geochemical and mineralogical point of view, the high adsorption capacity of clay minerals adds to the effect of low hydraulic conductivities by greatly increasing the retardation of radionuclides and other contaminants, making clays ideal where isolation from the biosphere is desired. While the low permeability and high adsorption capacity of clay minerals are widely acknowledged, it is clear nonetheless that there is a need for an improved understanding of how the chemical and mineralogical properties of clay rocks impacts transport through them. It is at the pore-scale that the chemical properties of clay minerals become important since their electrostatic properties can play a large role (1). The negative electrostatic potential field at the clay mineral surfaces results in the presence of porosity domains where electroneutrality is not achieved: cations are attracted by the surfaces while anions are repulsed from them, resulting in the presence of a diffuse ion swarm – or diffuse layer. Numerical methods for modeling diffusion processes in clay media with the consideration of the presence of a diffuse ion swarm have met a growing interest in diverse communities in the past years. Information on cation and anions diffusivity has been sought at the molecular level for the smallest pore sizes, i.e. the interlayer nanopores (2,3), and this information has been used to draw a consistent picture of diffusion processes at the mesoscale using up-scaling approaches and pore-scale modeling techniques, such as random-walk and pore network models. These modeling approaches are, however, not yet applicable to the modeling of “laboratory scale” experiments, such as flow-through diffusion experiments, or to large temporal and spatial scale modeling exercise where numerous coupling with the materials reactivity must also be taken into account. In this respect, reactive transport modeling approaches have the significant advantage to be able to handle complex geometries and chemistry, heterogeneities and transient conditions. In this presentation, we will highlights recent developments of reactive transport modeling that makes it possible to tackle problems on diffusion processes coupled to geochemical reactions at the continuum and the micro-continuum scale.

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Dissolution-precipitation processes in tank experiments: an experimental benchmark and modelling strategies

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Dissolution-precipitation processes in tank experiments: an experimental benchmark and modelling strategies. J. Poonoosamy 1, 2, G. Kosakowski 1, E. Curti 1, N. I. Prasianakis 1 1 Laboratory for Waste Management, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland 2 present address: Institute of Energy and Climate Research (IEK-6) Nuclear Waste Management and Reactor Safety, Research Centre Jülich GmbH, 52425 Jülich, Germany

The evolution of porosity due to dissolution/precipitation processes of minerals and the associated change of transport parameters are of major interest for natural geological environments and engineered underground structures. We designed a reproducible and fast to conduct quasi 2D experiment to investigate kinetically controlled dissolution/precipitation reactions causing porosity changes (Poonoosamy et al., 2015). A quasi 2D Plexiglas tank of dimension 10 × 10 × 1 cm was filled with sand. In the middle of the tank we placed a vertically oriented 1 cm thick reactive layer consisting of a bimodal grain size distribution of celestite ($SrSO_4$) crystals. A barium chloride solution was injected into the tank causing an asymmetric flow field to develop. As the barium chloride reached the celestite region, dissolution of celestite was initiated and barite precipitated. Due to the higher molar volume of barite, its precipitation caused a porosity decrease and thus also a decrease in the permeability of the porous medium. The change of flow in space and time was observed via injection of conservative tracers, fluid pressure measurements and analysis of effluents. In addition, an extensive post-mortem analysis of the reacted medium was conducted. We could successfully model the flow and the transport of conservative tracers with a (continuum scale) reactive transport model. The prediction of the reactive experiments initially failed. Only the inclusion of information from post-mortem analysis gave a satisfactory match. In a next phase we refined the post-mortem analysis and concentrated on investigating the dissolution/precipitation mechanisms at the pore scale (Poonoosamy et al., 2016). Our analytical techniques combined scanning electron microscopy (SEM) and synchrotron X-ray micro-diffraction/micro-fluorescence performed at the XAS beamline (Swiss Light Source). The newly formed phases include an epitaxial growth of barite micro-crystals on large celestite and a nano-crystalline barite phase resulting from the dissolution of small celestite crystals with residues of celestite crystals in the pore interstices. Classical nucleation theory, using well-established and estimated parameters describing barite precipitation, was applied to explain the mineralogical changes occurring in our system. Our pore scale investigation showed the limits of the continuum scale reactive transport model. Although kinetic effects were implemented by fixing two distinct rates for the dissolution of large and small celestite crystals, instantaneous precipitation of barite was assumed as soon as oversaturation occurred. Precipitation kinetics, passivation of large celestite crystals and metastability of supersaturated solutions, i.e. the conditions under which nucleation cannot occur despite high supersaturation, were neglected. The insight gained from microscopic investigations suggested that a pore scale model that describes precipitation and dissolution of crystals at the pore scale for various transport and chemical conditions can increase our predictive capabilities. Pore scale modelling can be used to parameterize constitutive equations to introduce pore-scale

corrections into macroscopic (continuum) reactive transport models. Lattice Boltzmann reactive transport modelling equipped with nucleation kinetics sub-lattice modelling reproduces most of the observed processes at a large range of supersaturation states. Microscopic understanding of the system is fundamental for bridging the pore and the continuum scale.

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Imaging a pore network in a clay rock at the sub nanometer scale

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Clayey rocks properties are the focus of an ever-increasing interest from the geoscience community. These fine-grained sedimentary rocks (mudstone, argillite, shales etc.) are recognized as key-components for energy-related technologies, for which they could serve as isolation material (in radioactive waste disposal), caprocks (in CO2 capture and storage systems), or as reservoir rocks for hydrocarbons (gas and oil shales) (Bourg, 2015; Tournassat et al., 2015b). For all of these applications, accurate predictions of mechanical, flow, and reactive properties at the field scale are necessary. However, macroscale properties of clayey rocks arise for a large part from the surface properties of their nano-sized clay minerals constituents and from the characteristics of associated microstructure and pore network. Pore networks in clayey rocks are highly heterogeneous with pore widths/diameters ranging in the categories of micropores (< 2 nm), mesopores (> 2 nm and < 50 nm) and macropores (> 50 nm). The fact that the pore size distribution in clayey rocks encompasses all of these pore size categories evinces the multiplicity of coupled physical processes that must be taken into account to explain observations at the core and field scales. Even if, FIB-SEM has enabled to improve the nanoscale characterization up to 5 nm (Gaboreau et al.,2016) must of the smallest pores, ensuring the connectivity, are not probed at this scale. One of the biggest challenges in the present downscaling approaches is a lack of understanding of the pore structure down to the (sub)nanometer pore sizes, which can contain up to 30 % of the total porosity, and which is also hypothesized to ensure most of the connectivity between bigger pores (Ma et al., 2016). In this study, we imaged in three dimensions the structure of a clayey rock down to the sub-nanometer scale using electron tomography. Pore network connectivity was extracted at the nanometer scale, providing key information for the building of future pore scale models.

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Investigation of the influence of surface roughness on geochemical reaction rates in fractures

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In most complex Earth and environmental systems, grain or fracture surfaces are not smooth. The presence of roughness not only increases surface areas beyond what would be calculated based on the assumption of an ideal geometry, but it also affects the local hydrodynamics and the accessibility of mineral surface area for reaction. Consequently, roughness may contribute to the discrepancy between reaction rates measured in the lab and those measured in the field [White and Brantley, 2003]. The impacts of surface roughness on reaction rate also need to be considered for more accurate parameterization of continuum scale reactive transport models. Reactive transport models at the continuum scale are essential in the investigation of the interactions between geochemistry and hydrodynamics within many natural and engineered systems, such as geologic carbon storage reservoirs and the critical zone [Steefel et al., 2005]. In the modeling, average properties (e.g. reaction rate) are commonly used to implicitly account for sub-grid heterogeneities, such as those that arise from surface roughness. While the impacts of surface roughness on average reaction rate are commonly accounted for through adjusting surface area, how roughness affect hydrodynamics and accessibility of reactive surface area has not been extensively investigated. In order to examine the conditions under which surface roughness affects reaction rate within a given pore or fracture segment, we conducted pore-scale reactive transport modeling based on 2-D domains with rough surfaces using Chombo-Crunch [Molins et al., 2012]. For the simulations, the rough surfaces are generated by superimposing a series of sine waves such that they are statistically representative of the rough fracture surfaces observed in natural systems. A range of velocities and reactions are investigated. The simulation results show that accounting for the surface area change caused by roughness alone cannot capture the impacts of roughness on reaction rate under the following conditions. At the high velocities, re-circulation zones may develop and reduce the accessibility of reactive surface area. At velocities that are slow relative to reactions, local equilibrium may develop and suppress the overall reaction. For a given velocity, the extent of the impacts of roughness on local hydrodynamics and therefore reaction rate appears to be related to the roughness measurement, indicating the potential of constructing phenomenological laws to fully account for the impacts of surface roughness on reaction rate.

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Mechanical and chemical effects of capillarity in macrovolume: Experimental evidences

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Porous rock in contact with atmosphere (exposed rocks, building materials, deep aquifers dried by drilling operations) is highly sensitive to relative humidity and temperature variations. Successive wetting – drainage stages result in phase transitions that generate perturbations of mechanical and chemical balance in porous media. In particular, crystallization of salts is recognized as one of the major causes of rocks and building disintegration. In drying conditions, poral solution is brought into a capillary state that decreases liquid pressure, reaching negative values in nanometric pores. Yet, the thermodynamic (Mercury and Tardy 2001; Mercury et al., 2003; Lassin et al., 2005; 2016) and mechanical (Tas et al., 2003) consequences of capillarity is usually ignored because the corresponding volumes are limited to nanometer pores (Young-Laplace law). However, in porous systems combining outer nanopores and inner macropores, the capillary tension generated at the nano-throats can affect the enclosed macrovolume. This is what is called an ink bottle geometry studied in soil physics. We developed experiments to attempt to reproduce this poral geometry in microcapillaries, and observe any associated chemical and mechanical consequences. Borosilicate cylindral (200 µm ID) and square capillaries (400x400 µm square section) are filled with sodium chloride or sodium sulfate solution. Evaporation at room temperature and at 50% relative humidity allows the crystallization of two salt plugs entrapping saline solution (Fig 1). Tensile state of confined liquid is revealed by inward displacements of salt plugs (mechanical effect) as well as the nucleation of a gas bubble inside the macrovolume (Fig 2). Dissolution of salt and gases arises as long as the macrovolume is under capillary pressure, in agreement with thermodynamic calculations (Fig 2, closer view). Using our method, salt crystallization in microcapillaries forms the intended poral geometry, where a confined micropore is connected to outer nanopores. In drying condition, capillary state of the annular film around crystal induces a superheated state in the macrovolume that establishes new solid-liquid-gas chemical and mechanical equilibria. These results show that capillarity can have a significant role in solid-liquid-gas interactions in natural porous media, whenever the properties of equilibrated capillary menisci are transmitted to macrovolumes.

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Micro-Continuum Approaches for Modeling Pore Scale Reactive Transport

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We introduce a micro-continuum modeling approach that builds on high resolution microscopic imaging that can be used to investigate the extent to which the 3-5 orders of magnitude lab-field discrepancy is due to porous media effects. The approach is applied to the study carbonate mineral trapping rates in the lower Tuscaloosa Formation at the Cranfield pilot injection site in Mississippi. Bulk reaction rates in the heterogeneous sediment are estimated by carrying out 2-D diffusion-reaction simulations using volume averaged porosity and mineral distributions determined based on 2-D Back Scattered Electron Scanning Electron Microscopy (BSE-SEM mapping.. The 2-D BSE-SEM data was augmented by 35 nm resolution FIB-SEM characterization of nano-porous chlorite zones, which was then used as the basis for numerical simulations to estimate effective diffusion coefficients for the chlorite-rich zones. The sparse distribution, limited connectivity, and low diffusivity of chlorite in the sediment all contribute to the low bulk reactivity of the sandstone. A second effort involves the interpretation of detailed characterization data from the Nagaoka Formation in Japan, the site of a pilot CO2 injection field experiment. In this study, a range of reactive surface area estimates were developed and evaluated for their ability to predict dissolution rates in well stirred and intact core reactor experiments. Reactive transport modeling was used to determine which of a number of reactive surface area models provide the best match with the effluent chemistry. The closest match with the well-stirred experiment were obtained by using specific surface area estimates from a newly developed image-based approach, while the porosity accessible reactive surface area (10 to 20X lower) provides the best match to the intact core data.

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Model Analyses Related to Groundwater Remediation

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Model analyses of groundwater remediation scenarios frequently fail because the probability of adverse, unanticipated events occurring is often high. This is driven by many factors including that (1) the models developed to represent the flow and transport in contaminated aquifers are typically simpler than reality and do not account for all the important governing processes (e.g. do not account for pore-scale processes), (2) probability distributions are assigned to critical performance parameters (such as model inputs or characteristics of the engineered remediation systems) even though some of these parameters might be unknown or not be very well constrained. We demonstrate model analyses evaluating uncertainties in model predictions caused by these factors. We also discuss how these uncertainties impact remediation decision analyses for a series of synthetic problems that are designed to be consistent with real-world problems. We also discuss a general computational framework for model and decision analyses: MADS (http://mads.lanl.gov and http://madsjulia.github.io/Mads.jl).

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multi-scale modeling of dynamics in clay/water systems

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Numerous experimental and theoretical studies have focused on predicting the performances of clay minerals as barrier materials in the containment of high-level radioative waste by evaluating the diffusion of mobile species in compacted, water-saturated Na- bentonites. One diffulty arises from the complex, multi-porosity structure of clay materials. Molecular dynamics simulations, which describe the evolution of matter at the atomic scale, allow to access adsorption properties at the surface of the clay layer. Ions and water molecules show relative different behaviors at the interface. In any case, the presence of the clay surface induces a slowing down of the mobile species, with diffusion mechanisms different from bulk aqueous solutions [1-3], which can be compared with neutron diffusion measurements. If this type of simulations is helpful to understand the water/mineral interactions in detail and interpret experiments at the same scale, it is limited to ideal systems with relatively small dimensions. However in a multiscale approach, we will show how the values of the results obtained from molecular dynamics simulations can be directly used in Brownian dynamics simulations to simulate the diffusion of tracers (water and ions) through a micrometric clay sample with a complex multiporous structure.

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Multiscale characterization of carbonate rock deformation due to dissolution, precipitation, and compaction during core flooding of reactive fluid

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Geomaterials containing nano-pores (e.g., carbonate rocks and shale) have become increasingly important for emerging problems such as geologic storage of CO2, unconventional gas and oil recovery, enhanced oil recovery, and nuclear waste disposal. The coupling of geochemical reactions with hydrological and mechanical processes in nano-porous geomaterials can lead to complex behaviors involving the change of pore topology (e.g., precipitation, dissolution, compaction, fracturing) and mineralogy. As a result, these fluid-rock interactions can change hydrological, mechanical, and geophysical properties (e.g., permeability, rock strength, elastic, acoustic velocity) across spatial and temporal scales. In this work we characterize the impact of dissolution of calcite, precipitation of MgCO3, and mechanical compaction on the change of multiscale pore structures and mechanical properties. We used Liège chalk samples that have been flooded with MaCl2 in a triaxial cell for 516 days and 1072 days, respectively. The detailed description of chemo-mechanical processes in compacting carbonate rocks during a long-term testing is reported in Nermoen et al. (2015) and Zimmermann et al. (2015). We applied multiscale imaging and mechanical testing for identifying the impact of chemo-mechanical coupling on the change of mineralogy, pore-structure, and mechanical properties. The integrated multiscale imaging of carbonate rocks from nanometer to centimeter scales include dual focused ion beam-scanning electron microscopy (FIB-SEM), micro computed tomography (micro-CT), optical and confocal microscopy, 2D and 3D energy dispersive spectroscopy (EDS). First, we obtained 2D mineralogical mapping and pore structures over a large sample area (~ 0.4cm x 2cm) using EDS and optical microscopy, respectively, to determine the locations of FIB-SEM analysis. The mineralogical mapping reveals the interface of reaction front and the textural fabrics revealed by FIB-SEM images (i.e., 1000 image stacks) at 10 nm resolution and elemental mapping by 3D FIB-EDS at 10 nm resolution show alteration patterns due to dissolution, precipitation, and compaction compared to unaltered sample with clear grain boundary. FIB-SEM-EDS images of the altered sample at multiple locations show distinct pore features including discrete micro-cracks in the chemically unaltered zone, sharp precipitation boundaries in the chemically altered zone, and smooth and relatively large pore space in the boundary zone of chemical reaction. Nano-indentation testing at multiple scales will be performed to evaluate the impact of the change of pore structure and mineralogy on the mechanical property. Lattice Boltzmann simulations and several analyses of characteristics of pore structures are used to obtain permeability and multipoint statistics at several different scales. Overall, these results clearly demonstrate that it is very critical to characterize the change of multiscale pore structure associated with chemical reactions and mechanical deformation.

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Pore-scale and multi-scale models of geochemical evolution of fractures

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Understanding fracture evolution is essential for many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO2 sequestration, and geothermal energy extraction. Geochemical processes in particular play a significant role in the evolution of fractures through dissolution-driven widening, fines migration, and/or fracture sealing due to precipitation.

Conceptually, fractured systems have often been represented as being composed of fast flow paths -the fractures- and slow flow paths - the rock matrix. Darcy-scale continuum models have treated fractures as preferential flow paths with their permeability evolving as a function (often, a cubic law) of the fracture aperture. This approach has the limitation that it may oversimplify flow within the fracture and the geochemical reaction parameters as well-mixed conditions need be assumed in each grid cell of the model. In this talk, we will present two additional modeling approaches for fracture simulation based pore-scale and multi-scale concepts, respectively, and apply them to the simulation of experimental results of fractured dolomite core.

In the pore scale model, it is possible to resolve the fracture surface geometry explicitly in three dimensions and solve for flow and reactive transport within the pore space of the fracture. The model can capture the channelization of the flow path due to dissolution in transport limited conditions. However, even with high performance computing, the pore scale model is still limited in their ability to treat finer-scale heterogeneity that falls below the resolution of the discretization. For this reason, we extend the pore scale model to include a porous continuum that captures fine scale processes within the rock matrix while keeping a pore scale representation of the fracture itself. The resulting multi-scale model is capable to simulate flow and transport within 3D tortuous fracture geometry using a pore-scale approach and the development of a reacted porous matrix using a Darcy-scale approach. Computationally, both domains are connected via explicit flux matching across an interface represented by an embedded boundary in an structured mesh framework.

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Pore-scale simulation of mineral dissolution

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A micro-continuum approach is proposed to simulate the dissolution of solid minerals at the pore-scale. It relies on the Darcy-Brinkman-Stokes equation and locally averaged conservation laws combined with immersed boundary conditions for the chemical reaction at the solid surface [1]. The methodology compares well with Arbitrary-Lagrangian-Eulerian technique. The simulation framework is used to reproduce micromodel experiments of the dissolution of a single calcite crystal. The evolution of the calcite during the acidizing process is analyzed and related to flow conditions, i.e. Péclet and Damköhler numbers. Macroscopic laws for the dissolution rate are proposed by upscaling the pore-scale simulations. Finally, the emergence of wormholes during the injection of acid in the porous domain is discussed based on pore-scale simulations.

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Reactive surface areas in 1D and 2D RT simulations of the interaction between sedimentary rocks and CO2-rich waters

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In the context of the geological sequestration of CO2 we have performed a number of flow-through experiments (columns filled with crushed rock samples; Garcia-Rios et al., 2014; Davila et al., 2016a; Thaysen et al., 2016) and percolation experiments (artificially fractured cores; Garcia-Rios et al., 2015; Davila et al., 2016b, 2006c) in the laboratory. The rock samples were representative of the reservoir rocks (limestone and sandstone) and cap rocks (argillaceous limestone and marls) at the Hontomín site (Spain). In these experiments, acidic sulfate-rich solutions were injected into the columns. The composition of the outflowing solutions was continuously monitored and the reacted solids were analyzed after the end of the experiments. Different pCO2 conditions were implemented.

The CrunchFlow code (Steefel et al., 2015) was used for the 1D and 2D reactive transport modeling of the experiments. Model fit to the experimental observations was performed by adjusting the values of mineral surface areas, using reaction rate laws from the literature. Additionally, in the 2D simulations (fractured cores), diffusion coefficients in the rock matrix also had to be adjusted. An important result from the calculations was the extent of mineral reaction and porosity changes inside the columns. In general, the calcite surface area had to be diminished with respect to initial geometric values, which may be explained by transport control of the fast calcite dissolution. Different flow conditions also resulted in different values of the calcite surface area, reflecting different degrees of transport limitation. In contrast, the values for aluminosilicates (illite, clinochlore, albite) had to be increased, possibly due to differences in size, shape and surface roughness.

Accurate values of reactive surface areas, including transport control of fast reacting minerals (e.g. calcite), are important factors to take into account when trying to predict mineralogical and porosity changes during CO2 sequestration.

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Semi-analytical solutions and numerical approach for reactive transfer in a saturated pore network model

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Protection and remediation of ground water resources are a major societal challenge. It implies to understand the transport mechanisms of organic and inorganic pollutants in the saturated and unsaturated zones [1]. For that purpose numerous studies have been conducted to model the multiphase reactive transport in a porous media. At Darcy scale, the behavior of solutes depends on microscopic heterogeneity for the media. The Pore Network Models (PNM) simplify drastically its geometry and consider pores linked by straight throats of constant section [2]. With such geometry the solution of the Stokes'equation is directly integrated and the flow is given by a Poiseuille flow. The computational effort is dramatically reduced thanks to the main advantage of the PNM [3].

As chemical reactions are very sensitive to the reactant concentration it is important to be able to follow precisely their values [4] throughout the pore network. Using Laplace transform [5,6,7], the reaction-transport equation is integrated in throats based on the main assumption that pores act as perfect reactors. Furthermore, we exhibit a semi-analytical solution of the time evolution of the concentrations in both throats and pores. The solutes transport consists in a Volterra equation system. Its convolution kernels are expressed as a summation of exponentially decreasing time functions (except the first term which is constant). The time constant is driven by the diffusion time (td). As td goes to zero, keeping the Peclet number fixed, each term of the summation reduces to a Dirac. The response of the system is then instantaneous. When the volume of the pore is large enough it is possible to neglect all the terms of the kernel except the constant one. In the limit where the Peclet number goes to zero, usual models are recovered. Numerically, the exponential decay time of the kernel allows optimizing the computational time according to a given precision.

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Small Angle Neutron Analysis of the Effect of Weathering on the Multiscale Pore Structure of Granites

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The microstructure and evolution of pore space in sedimentary rocks is a critically important factor controlling fluid flow properties in geological formations, including the migration and retention of water, gas and hydrocarbons, sequestration of wastes, the formation of ore deposits, and the evolution of metamorphic terranes. The size, distribution and connectivity of these confined geometries collectively dictate how fluids migrate into and through these micro- and nanoenvironments, as well as wet and react with the solid surfaces. As noted by Navarre-Sitchler et al. (2013), pristine igneous bedrock does not usually contain significant water. However, infiltration of meteoric water causes the rock to begin to disaggregate into soil, releasing nutrients and increasing the porosity and surface area. These processes in turn form the substrate in which biota can be sustained. In many igneous rocks this process is enhanced by oxidation of the original mineralogy. However, the processes by which this forms porosity, breaking down the rock are poorly understood and we cannot accurately extrapolate laboratory reaction rates to the field in predictive numerical models. While there are many methods for interrogating pore structure, it is difficult to satisfactorily describe textural and porosity changes in rock samples using direct imaging techniques because of the wide variation in length scales involved. A combination of SANS and USANS is, however, well suited to this task (cf. Anovitz et al., 2009, 2013, 2015a,b; Anovitz and Cole, 2015). The weathering process in granite is especially complex. While more mafic rocks tend to alter diffusively, forming altered rims, stresses caused by oxidation of ferromagnesian minerals like biotites tend to cause granites to spall. In order to better understand the effects of oxidation on the weathering process we have performed a series of experiments on granite cores approximately 5/8” in diameter by 5/8” long. These have been reacted in a solution of Se6+ at 200°C for periods of 1, 2, 4, 8, 16, 32, 64, 256 and 438 days. The reaction of Se6+ to Se4+ is very oxidizing relative to that of the Fe2+ in the granite, the solution contained enough to buffer twice the ferrous iron expected in the rock sample, and no secondary phases are expected to form. Because of the geometry these are expected to form oxidized rims that grow with time prior to failure, and the reactive porosity and micro-stress-fractures are easily discernable and quantifiable by (U)SANS. This was analyzed using annular Cd masks to isolate core and rim processes. These were supplemented by SEM analyses. Results suggest that reactive stresses play a significant role in the evolution of porosity during weathering.

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Visualizing concentration distributions in macroscopic samples in the course of geochemical processes

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Geochemical processes, although generally well characterized on the molecular scale, are complicated by structural effects and process-inherent pattern formation. These effects cause variable scaling behaviour of the processes. This can be investigated through a significant process variable, the concentration of a geochemical species. As experimental method, therefore, we established positron emission tomography (PET) for high-resolving, sensitive, and quantitative tomographic imaging of tracer distributions in representative samples on the scale of drill cores (Kulenkampff et al. 2016). In contrast to other groups, we utilize a high-resolution PET-scanner and specially designed reconstruction software („GeoPET“) with about four times higher spatial resolution (about 1 mm) than standard medical PET scanners. This resolution is adequate for drill core sizes, and enables to visualize and analyze preferential pathway effects and local accumulations of tracers in detail, with an integration volume just above the typical pore scale. Thus, the method is ideally suited for parameterizing and verifying reactive transport simulations on the relevant macro-scale. We applied the method on a variety of reactive transport processes, including leaching of copper minerals, injection of water glass for barrier improvement, transport of plant protectants in the soil, and transport of nano-particles in soils, rocks and technical devices. Generally, both with conservative and reactive tracers, we observe strong localization of the transport pathways. This formation of preferential transport pathways implies that simulation models should consider a decrease of the effective volume and effective internal surface area, as well as high concentration gradients and non-uniform concentration distributions. PET is the potential method for parameterizing such models without prior flow simulations based on tomographic modalities for structural imaging, like µCT.

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A Lagrangian transport Eulerian reaction spatial (LATERS) Markov model for prediction of effective bimolecular reactive transport

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Predicting chemical reactions in porous media can be challenging due to the complex and non-uniform nature of flows at pore scales [1]. One of the most obvious but critical features to recognize in any reactive system is that for reactions to occur, the reactants involved must physically come into contact with one another via mixing. When the flow is complex, prediction of mixing can be challenging, particularly if one desires to make predictions at scales larger than the pore scale, requiring an upscaled modeling framework. Accurate modeling of mixing is best done in a Lagrangian framework, particularly at early times, while efficiently modeling reactions is best done in an Eulerian framework. So we propose to do just that. An upscaled Eulerian model of bimolecular reactive transport was developed by Porta, et al.[2], which results from volume averaging of the advection diffusion reaction equation. The usual closure for this model is Eulerian as well, but we propose a Lagrangian closure, based on the Spatial Markov model [3]. The hybrid model we propose is a LAgrangian Transport Eulerian Reaction Spatial Markov model (LATERS Markov model), which uses an extension of the Lagrangian Spatial Markov model, developed by [3], to transport particles, then maps their positions to an Eulerian grid to simulate reactions using the volume averaged reaction term in [2]. The advantage of this approach is that the Spatial Markov model is known to provide accurate predictions of transport, particularly at early times, when transport is more difficult to model, and Eulerian reaction method is efficient, because it does not require calculation of distances between particles. This presentation introduces the LATERS Markov model and demonstrates its ability to predict bimolecular reactive transport in a simple 2D porous medium made of a regular array of circles.

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Anomalous reactive transport in porous media: Experiments and modeling

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We analyze dynamic behavior of chemically-reactive species in a porous medium, subject to anomalous transport. In this context, we first present transport experiments in a refraction indexmatched, three-dimensional, water-saturated porous medium, using a pH indicator as a reactive tracer to follow chemical reactions. The porous medium consisted of a novel acrylic polymer material formed as spherical beads that have pH buffering capacity. The magnitude of reaction during transport through the porous medium was related to the color change of the pH indicator, via image analysis. Here, we focused on point injection of the tracer into a macroscopically uniform flow field containing water at a pH different from that of the injected tracer. The set-up yielded measurements of the temporally evolving spatial (local-in-space) concentration field. Parallel experiments with the same tracer, but without reactions (no changes in pH), enabled identification of the transport itself to be anomalous ("non-Fickian"); this was quantified by a continuous time random walk (CTRW) formulation. A CTRW particle tracking model was then used to quantify the spatial and temporal migration of both the conservative and reactive tracer plumes. Model parameters related to the anomalous transport were determined from the conservative tracer experiments. An additional term accounting for chemical reaction was established solely from analysis of the reactant concentrations, and significantly, no other fitting parameters were required. The measurements and analysis emphasized the localized nature of reaction, caused by small-scale concentration fluctuations and preferential pathways. In addition, an "threshold radius" for pH-controlled reactive transport processes was defined under buffering conditions, which delineated the region in which reactions occurred rapidly.

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Controlling Water Production by Application of Smart Well Technology

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Abstract (Max 500 Words): Water injection has been one of the most effective methods to improve oil recovery as it can be used to maintain the reservoir pressure or improve fluid flow movement in reservoir. The success of water injection projects depends on postponing or preventing water breakthrough from production wells which might happens so quickly in the multilayered and heterogeneous reservoirs. The oil recovery factor can be improved by monitoring and controlling the fluid flow of both injection and production networks through those of reservoirs. Downhole interval control valves (ICVs) allow to control unconventional wells efficiently, even in the heterogeneous reservoirs. These wells called smart wells, provide the ability to independently control each perforated layer in real time. The smart wells allow to maximize the oil production or to minimize unwanted fluid production by monitoring and controlling the fluid flow without intervention. This paper aims to study the application of intelligent wells and IPM suit and to investigate the production and EOR scenarios in order to improve oil recovery and postpone the water breakthrough. In this paper, one heterogeneous and multilayered oil reservoir under water injection operation was investigated. Integrated Production Modelling (IPM) is employed to design smart wells (ICVs). Then, this integrated intelligent reservoir model was examined to manage oil production rate as well as water injection rate under field constraints to improve reservoir production performance. In this regard, several reactive and proactive scenarios were studied and the optimal scenario which maximized the oil recovery was identified. The results demonstrated that employing smart completions (ICVs) through IPM approach significantly increased the oil recovery by controlling the fluid flow. Besides, in order to decrease the water production and enhance production revenue, the smart completions were applied through injection wells. According to the results, the use of smart well equipment (ICV) in the injection wells and implementation of the best Reactive and Proactive scenarios using smart well technology can significantly reduce the water production and as a result increase the oil recovery.

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Coupling of mixing and kinetic limitations in reaction front dynamics

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Mixing fronts, where fluids of different chemical compositions mix with each other, are known to represent hotspots of chemical reaction in hydrological systems. These fronts are typically subjected to velocity gradients, ranging from the pore scale due to no slip boundary conditions at fluid solid interfaces, to the Darcy scale due to permeability variations. A common trait of these processes is that the mixing interface is strained by shear. Depending on the P{\'e}clet number $\textsf{Pe}$, which represents the ratio of the characteristic diffusion time to the characteristic shear time, and the Damk{\"o}hler number $\textsf{Da}$, which represents the ratio of the characteristic diffusion time to the characteristic reaction time, the local reaction rates can be strongly impacted by the dynamics of the mixing interface.

Here we investigate the coupling of fluid deformation and chemical reactivity for arbitrary Damk{\"o}hler numbers, for an initial interface with separated reactants. Approximate analytical expressions for the global production rate and reactive mixing scale are derived based on a reactive lamella approach that allows for a general coupling between stretching enhanced mixing and chemical reactions. While for $\textsf{Pe}<\textsf{Da}$, reaction kinetics and stretching effects are decoupled, a scenario which we name "weak stretching", for $\textsf{Pe}>\textsf{Da}$, we uncover a "strong stretching" scenario where new scaling laws emerge from the interplay between reaction kinetics, diffusion, and stretching.

The obtained analytical results are validated against numerical simulations and micromodel experiments based on chemi-luminescence. For the latter, we adapted the setup of de Anna et al. (2014) to tune the reaction constant and explore a range of Damkohler numbers. These findings shed light on the effect of flow heterogeneity on the enhancement of chemical reaction and the creation of spatially localized hotspots of reactivity for a broad range of systems ranging from kinetic limited to mixing limited situations.

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Effects of incomplete mixing on chemical reactions under flow heterogeneities.

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Evaluation of the mixing process in aquifers is of primary importance when assessing attenuation of pollutants. Mixing processes control biogeochemical transformations such as precipitation/dissolution or degradation reactions that are fast compared to mass transfer processes. Reactions are local phenomena that fluctuate at the pore scale, but predictions are often made at much larger scales. However, heterogeneities are found at all scales and create complex concentration distributions that enhances mixing. In order to quantify the effects of mixing on mixing-controlled reactions, we study a bimolecular irreversible chemical reaction A + B → C. We use a reactive random walk particle tracking (RWPT) method to simulate bimolecular reactive transport experiments. Our numerical approach represents the reactants by particles and the molecular diffusion and the reaction rate constant dictate the reactions. To assess the impacts of flow heterogeneities at pore scale, we model the chemical reaction under two different flow regimes. First, we focus on the experimental scenario by Gramling et. al (2002). These authors studied the reactive displacement of B by A in a Darcy-scale homogeneous medium and found that the Darcy-scale theory overpredicts the amount of reaction product formed. This discrepancy is traced back to pore-scale velocity fluctuations. We model these velocity fluctuations in our reactive RWPT model by an Ornstein-Uhlenbeck velocity process to represent incomplete mixing on the pore scale. Second, we analyse the irreversible bimolecular reaction for a laminar Poiseuille flow reactor to study and quantify the impacts of flow variability in a single pore. We observe three different time regimes characterized by different behaviours of the product formation. At early times, pre-asymptotic regime, mixing is dominated by diffusion. For times larger than $\tau v = 2D/(v^2)$, after which advection begins to dominate over diffusion, we find enhanced reaction efficiency due to flow variability. Finally, for times larger than the characteristic time of diffusion (τD), asymptotic regime, we find that mixing is represented by the Taylor dispersion coefficient.

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Flow and transport in a 2D wavy channel of randomly varying aperture

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Our work deals with the investigation of fluid flow and solute transport in channels of randomly varying apertures: the study of this problem is relevant to many direct practical applications in systems both natural, as fractured geological formations, and engineered, as microfluidics devices. The existing works dealing with transport in channels with non-constant diameter are limited to periodically varying apertures [1] or small-scale roughness in pipes [2]: the available literature indicates non-trivial effects on apparent mechanical dispersion resulting from variations in channel apertures, but a full description of the problem considering the range of variation of the geometrical features of realistic systems is still missing. The aim of the current study is thus to improve on the current understanding of these effects, specifically by studying the influence of randomness in the channel size. In our approach, we build a suitable number of geometric realizations of 2D channels with sinusoidally varying apertures of random amplitude and random channel diameter: a detail of the geometry can be seen in Fig. 1. Then, flow field and particle transport are investigated by means of finite volume CFD simulations (using the open-source code OpenFOAM). First, flow field is obtained in Stokes regime, then the solute transport is studied via Lagrangian particle tracking, covering a very wide range of Péclet numbers. Values of permeability are calculated and related to variations in sinusoidal amplitude and channel diameter: preliminary results are shown in Fig. 2. Finally, values of solute dispersion are presented against variations in channel geometry. We observe marked differences compared with the classical Taylor-Aris solution for transport in pipes and the mentioned study on periodic channels: as such, the results of this work highlight the great impact of geometric configuration on both flow and transport.

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Fluid stretching in heterogeneous porous media as a coupled continuous time random walk

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We study the deformation of material fluid elements as they are moving in the flow through heterogeneous porous media. Material fluid elements can be seen as deformable support volumes (lamellae) for solute mixing and chemical reactions, which are determined by the local Lagrangian deformation behavior. Thus, stretching and compression of material fluid elements is a key element for the understanding and quantification of the mixing and reaction dynamics in heterogeneous porous media flows from the pore to the Darcy scale. The compression of fluid lamellae due to the stirring action of the flow field steepens concentration gradients and leads to enhanced diffusive solute fluxes and thus enhanced mixing and dilution. Linear and exponential in time elongation behaviors are typical for shear flows and chaotic flows, respectively. For porous media flows one typically observes algebraic stretchings characterized by sub- or superlinear elongations and in general sub-exponential behaviors. These behaviors can be traced back to intermittent shear events experienced by material fluid elements as they move along a streamline. In order to systematically quantify these behaviors, we cast the fluid deformation problem in streamline coordinates. Explicit analytical expressions for the Lagrangian deformation tensor show that fluid elongation is fully determined by the Lagrangian velocity series and shear rate along a streamline. We find find that intermittent episodes of increased fluid stretching are related to zones of low flow velocities, whose extension is of the order of the characteristic heterogeneity scale. These behaviors are quantified systematically by modeling Lagrangian velocities and thus deformation as a stochastic process that evolves in equidistant spatial steps along streamlines [1, 2]. This leads to a description of fluid particle motion in terms of a continuous time random walk (CTRW) whose time increment is given kinematically by the distance traveled divided by the particle velocity. The deformation increment is a function of the particle velocities and thus coupled to the time increment. This leads us naturally to the description of the stretching process as a coupled CTRW. We use this framework to derive subexponential stretching behaviors and relate them to the Eulerian velocity distribution and flow organization [1, 2]. We apply the derived framework to Darcy-scale flow in heterogeneous conductivity fields and determine the elongation statistics in terms of probability density function of elongation and the evolution of its mean. Furthermore, we investigate the interactions of these stretching dynamics with diffusion for the evolution of solute blob.

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Increasing the Order of Collocation Methods — Equivalence Between Lagrangian and Eulerian Formulations of Multicomponent Reactive Systems

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Reactions involving multiple chemical species occur in countless natural and engineered systems of interest. It is well known that the well-mixed formulation, which assumes perfect mixing of all chemical components at every moment in time, often fails to capture the observed behavior, due to local depletion of some of the reaction elements which cannot be instantaneously compensated by the transport mechanism. The Advection Dispersion Reaction Equation (ADRE) is often used to model the combined effect of transport and local mass-action-law reactions. Traditionally, Eulerian methods are the tools of choice to solve this equation numerically. While they are well understood, they often suffer from numerical dispersion, which leads to overprediction of mixing and therefore reactions. In order to circumvent this problem, high order methods with fine discretizations are often needed, incurring high computational costs. Conversely, Lagrangian random walk methods are less prone to numerical dispersion, but their convergence properties are less well understood. In this presentation, I will show the equivalence between the ADRE and a Lagrangian random walk method relying on a collocation probability formulation for a multispecies annihilation reaction. I will then show how the temporal and/or spatial accuracy of the method may be increased beyond the currently standard first order methods.

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Modeling Heterogeneous Reaction by Random Walk Simulation

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Random Walk (RW) models are a Lagrangian type numerical models which can be very successful in modeling transport of sharp concentration fronts. The treatment of first-order kinetic reactions A->B by RW models is relatively straightforward and has been developed almost 3 decades ago. In recent years, new RW models have been developed to tackle second order kinetic homogeneous reaction A+B->C with a given rate constant [Paster et al. 2013,2014,2015]. In such models the A,B particles have a probability to annihilate each other. That probability is a function of the distance between the particles, the diffusion coefficient, and the time step size (i.e. time discretization). So far, RW models were unable to tackle heterogeneous reactions, i.e. reactions happening over a surface. Such reactions are common in chemical engineering practice, e.g. packed bed reactors where a catalyst is doped over the surface area of the porous material. In such cases, if the problem is modeled at the pore scale, the boundary condition for transport reads -DdC/dx=kC at the surface. Here, k is a rate constant for the surface reaction. As mentioned above, present RW models are unable to tackle this boundary condition. The current study aims to fill this gap, by presenting a new model for heterogeneous reactions. We apply the boundary condition at the reactive wall as follows: (1) All particles that hit the wall during a time step are reflected, and (2) a fraction of the reflected particles are annihilated. This fraction (i.e. annihilation probability) is a function of the reaction rate and the size of the time step. An analytical expression for the annihilation probability is developed and tested for simple cases. We apply the approach for modeling a specific experiment of photocatalytic reaction on the surface of a porous media (alumina (Al2O3) 800 nm microfiltration membrane, with N-doped TiO2 sol-gel thin film deposition). In this experiment, the membrane is placed under a solar simulator and illuminated from top. Water with known concentration of viruses is pumped through the membrane in a dead-end filtration mode. Light irradiation hits the catalyst at the surface of the porous media and OH (hydroxyl) radicals produced result in photocatalytic oxidation of reactants on or near the surface. This technology is under consideration as a relatively low-cost and environmentally viable alternative for purifying water as it exploits solar irradiation and due to the simplicity of applying coating on a commercially available ceramic membrane. For simplicity we model the porous media as a bundle of tubes of uniform diameter (the pore scale of the porous media). We apply the RW approach to these tubes and evaluate the survival probability of contaminants that travel through the membrane. By comparing the model results to experimental virus inactivation results, we evaluate k for the membrane. Then, we use the model to investigate how the membrane pore size and discharge rate effect the efficiency of the system.

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Modeling of adsorption with particle tracking and kernel density estimators

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Adsorption, the binding of atoms or molecules from a gas or liquid to a surface, is a phenomenon in many physical, biological, and chemical systems and processes. To design and optimize an adsorption-based process, it is necessary to characterize accurately the adsorption equilibria and their dependence on the experimental conditions. We have recently developed a model based on Particle Tracking Methods (PTM) and Kernel Density Estimators (KDE) that can be directly used to study bimolecular reaction in diffusive problems [1]. The main idea is to use Kernels to provide new weighting functions for particles to interact. In this case, when particles are transformed into another species or mineral, the shape of the Kernel automatically adjusts, expanding its region of influence and the region of interaction between particles. This feature is beneficial to avoid incomplete mixing due to the segregation of particles. Here, we extend this model for simulating nonlinear adsorption. By introducing homogeneous and inhomogeneous distributions of adsorption energy in our model, we simulate the classical Langmuir and Freundlich isotherms for predicting an adsorption-based process. Simulation results show a good agreement with the analytical results of the Langmuir model even with a low number of particles. The mono-layer adsorption (saturation) is also observed due to the limited number of adsorbent sites. Following the Freundlich isotherm, we find a good agreement between the logarithmic slope of the adsorbate-adsorbent concentration and the Freundlich constant for low adsorbate concentrations. The saturation of adsorbent sites is also observed for high concentrations, pointing out the ability of our model to combine the features of the classical Langmuir and Freundlich isotherms. Our proposed approach opens up a new way to predict and control an adsorption-based process using a particle-based method with a finite number of particles.

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Modelling bimolecular reactions involving complex kinetics via particle tracking

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In recent years a large body of literature has been devoted to study reactive transport of solutes in porous media based on pure Lagrangian formulations. Such approaches have also been extended to accommodate bimolecular reactions provided the kinetic term can be written as proportional to the product of the concentration of the two reactants. Rather, in some cases, reactive transport in bimolecular reactions involves more complicated rate laws that are not linear with respect to the concentration of the reactants. Some examples are (1) reaction rate laws written in terms of powers of concentrations, (2) redox reactions following a Michaelis-Menten rate law, or (3) any reaction where the activity coefficients vary with the concentration of the reactants, just to name a few. We provide a methodology to account for non-linear reactions in a fully Lagrangian approach where each particle represents an amount of mass of a specific solute. The method, built as an extension to the first-order case, is based on the concept of optimal Kernel Density Estimator, which allows the concentrations to be written in terms of particle locations hence transferring the concept of reaction rate to particle location distribution. By doing so, we can update the probability of particles reacting without the need to reconstruct the concentration maps. The methodology is implemented in a 1D model to reproduce the Advection-Dispersion-Reaction Equation (ADRE), and its performance is tested for several hypothetical case examples. The results show convergence towards the finite-difference solution as the number of particles is increased.

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Multiscale methods for unresolved pore-scale heterogenous samples

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Multiscale methods with different degrees of coupling require detailed information about the pore topology wherever pore-scale models are resolved. While X-ray computed tomography (XCT) images of natural geological porous media columns are generally considered the ground truth for a detailed description of the pore-scale structure, microporosity in heterogenous geological samples if often below the instrument resolution. This unresolved porosity has dramatic effects on the predictive capabilities of pore- and/or multiscale models based on standard threshold-based segmentation algorithms. We develop a novel efficient algorithm of downscaling followed by segmentation to reconstruct the unresolved pore space from X-ray computed tomography (XCT) images of natural geological porous media columns. The method allows transformation of poorly resolved gray-scale images of a highly heterogeneous porous sample into high-resolution binary images while preserving important sub-resolution information. The method maps pixel intensity into pore-space and matches the total porosity of the high-resolution binary image with the total porosity of the porous medium. After the downscaling, the binary image is segmented into interconnected void regions bounded by the solid phase, where each region corresponds to a single pore. We apply the method to extract the pore space distribution from unresolved XCT images of two natural sediment columns and we estimate the hydraulic conductivity and breakthrough behavior of the solute transport and compare with the experimental data. The comparison demonstrates that the algorithm is accurate and the model predictive across multiple length scales.

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Simulation of complex geochemistry in the Lagrangian reference frame

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Simulation techniques for reactive transport systems have advanced greatly in recent years, but the majority of studies still require a tradeoff in complexity. This tradeoff may place attention on the detailed geochemical reaction process by simplifying physical transport and mixing processes, or the opposite tradeoff. To date, the only studies that have incorporated realistic aspects of both have been Eulerian and these have still simplified representations of mixing processes. This presentation describes a Lagrangian technique for simulating complex geochemistry that minimizes assumptions about the mixing state over time. The core of the approach is the particle colocation framework [Benson and Meerschaert, 2008; Bolster et al., 2015] but it is adapted to multi-species, multi-step reactions. The new approach assigns multiple component masses to each particle but diffusion allows mass to be exchanged between the particles using the colocation density as the mass transfer rate. After the mass exchange step, the geochemistry of each particle is at a state of disequilibrium and the reaction engine PhreeqcRM [Parkhurst and Wissmeier, 2015] is used to relax the geochemistry toward equilibrium. The approach is first validated against several well-known analytical solutions and experimental results of reversible and irreversible kinetic and equilibrium reactions. We then move on to a comparison of multi-step reactions in a diffusive system where the traditional PHREEQC model is used for cross-validation. Finally, we highlight the capabilities of the new approach with examples of completive reactions, incomplete mixing in complex geochemical systems, and the effects of heterogeneous distributions of reaction sites on upscaled reaction rates.

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The impact of mass transfer limitations and heterogeneity contrasts on the parameterization of longitudinal dispersion in numerical models

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A challenge in modeling solute transport in groundwater is how to parameterize hydrodynamic dispersion and which values to assign to coefficients in the blocks representing grid cells of a numerical model. Actual geologic formations are heterogeneous at all scales but numerical models resolve only larger scale heterogeneity by considering blocks with different parameters, while heterogeneity at scales smaller than the size of blocks is not explicitly resolved. Dispersion coefficients originate from the joint variability of velocities and solute concentrations at the small grain scale and at heterogeneity scales that are not resolved in the continuum description of solute transport within a given block. In this study we focus on the longitudinal dispersion coefficient and, starting from accurate local scale description of solute transport, we apply an Eulerian approach for computing the values of longitudinal dispersion coefficient to be assigned to numerical models' blocks. The method is valid under conditions of physical equilibrium for which dispersion is approximately Fickian (i.e., the dispersive flux is proportional to the gradient of the resolved concentration). The approach requires the solution of a steady-state advection-dispersion equation; it is computationally efficient, and applicable to any heterogeneous hydraulic conductivity field. In this work we consider binary heterogeneous media with a permeable matrix and distributed low-permeability inclusions. Numerical experiments where performed in blocks containing the same volume of low-permeability material but with different orientation, elongation and hydraulic conductivity contrast of the inclusions with respect to the permeable matrix (s2lnK=0.2-4.6). Multi-tracer simulations considering solutes with different aqueous diffusion coefficient were performed in a range of seepage velocity values spanning the conditions typical of groundwater transport problems. The results demonstrate the critical role of the interplay between advection and diffusion, as well as the importance of the heterogeneity contrast. In some cases characterized by low permeability contrast, small inclusions and fast seepage velocity, computed longitudinal dispersion coefficients for the considered blocks can be captured satisfactorily by the linear Scheidegger parameterization, using a constant dispersivity. However, when diffusive mass transfer plays an important role, non-linear and compound-specific parameterizations should be used to accurately calculate longitudinal dispersion coefficients in discretized numerical models. Implications of these findings for mixing-controlled reactive transport problems will also be discussed.

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Pore-scale reactive transport modeling of degradation processes in cementitious systems: Concept development based on the Lattice-Boltzmann approach

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Cementitious materials are used in a wide range of applications in nuclear waste management, for example for the solidification of waste or as construction and backfill material in underground and surface waste repositories. Some of the main reasons for their use are their low permeability and diffusivity and their properties with respect to radionuclide retention. Upon hydration, hardened cement paste is composed of cement hydrates such as C-S-H phases, portlandite, aluminate/ferrate compounds (AFm/AFt), porosity/porewater and unhydrated clinker. In cementitious materials, chemical and microstructural heterogeneities exist in a wide range of length scales (nm to cm). The macroscopic physical properties of these materials strongly depend on the pore structure and the (micro)structural and chemical changes resulting from long-term alteration/degradation processes. In this context, pore-scale reactive transport models can be regarded as promising tools to realistically describe the evolution of the pore structure and the heterogeneous distribution of hydrated phases in cementitious materials. Although the application of pore-scale models is relatively well established in other disciplines, applications to cement-based materials are only starting to emerge. The advantage of these models over traditional meso- and macro-scale models is their potential to reduce the level of empiricism of the current treatment of the coupling between chemical reactions and physical properties.

In the framework of the Horizon2020 collaborative project Cebama (Cement-based materials, properties, evolution, barrier functions) a pore-scale reactive transport model is under development and validation. The aim is to study the mass transport behaviour of cementitious materials and the impact of chemical degradation on its (radionuclide) transport properties. The focus is on degradation processes as a result of the interaction with different groundwater compositions (e.g. calcium leaching, carbonation or sulphate attack). For this purpose, a three dimensional (3D) advection-diffusion solver based on the Lattice Boltzmann Method (Palabos) has been coupled to a geochemical simulator (PhreeqcRM), using a dedicated interface. In this contribution, the authors present and discuss the modelling concept, the capabilities of the newly developed pore-scale reactive transport model, as well as the validation/benchmarking strategy. The latter is based on comparison of modeling results to analytical solutions as well as to experimental data and observations on concrete degradation processes.

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Coupled charge migration and fluid mixing in reactive fronts

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Quantifying fluid mixing in subsurface environments and its consequence on biogeochemical reactions is of paramount importance owing to its role in processes such as contaminant migration, aquifer remediation, CO2 sequestration or clogging processes, to name a few (Dentz et al. 2011). The presence of strong velocity gradients in porous media is expected to lead to enhanced diffusive mixing and augmented reaction rates (Le Borgne et al. 2014). Accurate in situ imaging of subsurface reactive solute transport and mixing remains to date a challenging proposition: the opacity of the medium prevents optical imaging and field methods based on tracer tests do not provide spatial information. Recently developed geophysical methods based on the temporal monitoring of electrical conductivity and polarization have shown promises for mapping and monitoring biogeochemical reactions in the subsurface although it remains challenging to decipher the multiple sources of electrical signals (e.g. Knight et al. 2010).

In this work, we explore the coupling between fluid mixing, reaction and charge migration in porous media to evaluate the potential of mapping the spatial distribution of reaction rates from electrical measurements. To this end, we develop a new theoretical framework based on a lamellar mixing model (Le Borgne et al. 2013) to quantify changes in electrical mobility induced by chemical reactions across mixing fronts. Electrical conductivity and induced polarization are strongly dependent on the concentration of ionic species, which in turn depend on the local reaction rates. Hence, our results suggest that variations in real and complex electrical conductivity may be quantitatively related to the mixing and reaction dynamics. Thus, the presented theory provides a novel upscaling framework to quantify the coupling between mixing, reaction and charge migration in heterogeneous porous media flows.

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Ion transport in weakly charged porous media and ion exchange membranes for shock electrodialysis desalination

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Shock Electrodialysis (shock-ED) is a novel technology to desalinate salt solutions by using ion exchange membranes (IEMs) and weakly charged porous media with the same polarity. The principle of shock-ED is based on the propagation of current-induced “deionization shocks” in porous media [1]. By applying an external voltage, a current runs through the membranes and across the porous medium, causing the propagation of deionization shock waves with a sharp boundary between concentrated and depleted zones. As a result, desalinated water and brine can be separated as outlet streams from a single channel [2]. Modeling the shock-ED process is a complex task, which requires the description of ion transport both in the membrane and in the charged porous medium. In particular, the role of co-ion flux is essential to understand transport phenomena in the porous medium (which acts as a “leaky” membrane in the system). Moreover, both transport of ions and fluid flow through membrane must be described in two dimensions, taking into account the Donnan potentials at each membrane-porous medium interface. In this work, we present a simplified steady-state model based on Nernst-Planck theory [3], in which the transport of both counterions and co-ions is fully described in the membrane and in the porous medium. Finally, we discuss perspectives for shock-ED, by identifying next research directions and promising applications.

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Microscale Simulation of the Impedance Spectroscopy Response of Rocks

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Understanding the Electrical Impedance Spectroscopy (EIS or IS) response of rocks is still a challenge even though many model approaches were published. For instance, Volkmann and Klitzsch (2010), Weller and Slater (2015), and Niu and Revil (2016) introduce recent numerical, semi-empirical, and analytical developments of IS models in geophysics, respectively. However, most of the models describing the IS response of rocks are based on simplified assumptions regarding both the microstructure and the physics of the processes at the rock-electrolyte interface. Moreover, the simulations of porous medium behaviour often treat the medium as homogeneous and link their material properties to microstructural properties by empirical equations.

Our goal is to develop an approach for numerically simulating IS of porous media that accounts for the real microstructure and the involved processes. Here, we present 1D and 2D time dependant IS simulations.

In porous media such as rocks or batteries, the interaction between electrolyte and solid material give rise to a charged solid surface and thus to the so called Electrical Double Layer (EDL) at their interface. The EDL arises in the electrolyte to compensate the charge of the solid surface; it consists of the Stern layer of counter-ions adsorbed to the solid surface and the diffuse layer with increasing concentration differences between cations and anions towards the solid surface. In the up to 1 kHz frequency range the EDL is the only cause for electrical polarization in rocks which do not contain electronic conductors.

The IS simulation module developed in MATLAB simulates the coupled diffusion and migration of charges in an electric field in the time domain. The involved processes are governed by the Nernst-Planck-Poisson (NPP) equations. As the first step, we performed nondimensionalization of the NPP model which provides better conditioning and is faster (i.e. lower iteration count) to solve with the iterative numerical solvers. The equations are discretized in space and time using the second order Finite Difference Method (FDM) and the first order Euler schemes.

In our approach, we model time domain IS in three steps: Step 1 - We simulated the steady state solution for the ionic concentrations and the potential distribution in an electrolyte around a solid particle carrying surface charges. Step 2 - In the next step, we simulated the steady state solution for the model above but applying an external potential across the model domain. Step 3 - After reaching equilibrium conditions, the external voltage source is switched off and the transient ion concentrations and potentials are calculated.

All in all, we simulate the time domain IS response of rock models by numerically solving the Nernst-Planck-Poisson (NPP) equations. We use the model for gaining a better understanding of the measured electrical spectra. For this, we carry out parameter studies, e.g, we investigate the influence of particle and pore size or of the solid's conductivity on the IS response.

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Modeling multicomponent ionic dispersion, electrochemical migration, and chemical reactions in porous media with IPhreeqc coupling

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Molecular diffusion and electrochemical migration are important processes affecting transport of charged species in porous media. In this work, we present a two-dimensional multicomponent reactive transport model taking into account the electrostatic interactions during transport of charged species in physically and chemically heterogeneous domains [1]. The modeling approach is based on the Nernst-Planck formulation and on the description of compound-specific and spatially variable diffusive/dispersive fluxes. The multicomponent ionic transport code is coupled with the geochemical code PHREEQC by utilizing the IPhreeqc module [2], thus enabling to perform the geochemical calculations included in the PHREEQC's reaction package. The multicomponent reactive transport code is benchmarked by comparing the model outcomes with the high-resolution experimental datasets obtained from controlled laboratory flow-through experiments. The experiments were performed in a quasi two-dimensional bench-scale setup, packed with water-saturated porous media, using dilute solutions of different strong electrolytes. The experimental results showed a remarkable influence of the charge interactions between the ionic species also in advection-dominated flow regimes [3]. The excellent agreement between the experimental results and the model simulations validates the proposed charge coupled diffusion/dispersion and electromigration calculations for macroscopic transport of charged species in porous media. Furthermore, we validated the 2-D multicomponent reactive transport code against 1-D PHREEQC simulations and we used the model to explore the effects of charge interactions in reactive transport scenarios in physically and chemically heterogeneous porous media.

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Multi-scale modeling of diffusion and electrochemical reaction for porous micro-electrodes

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Porous electrodes are of tremendous interest for numerous applications such as bisosensors, bioactuators, batteries… because of their high specific surface area that allows efficient rates of electrical energy production. Indeed, for a given over-potential, such electrodes may offer electrical current several orders of magnitude higher than classical flat electrodes of the same size [1, 2]. In this study, we develop a multi-scale model for transport and reaction in porous electrodes coupling electrochemical phenomena and diffusion mechanism in order to construct a macroscopic constitutive law that allows estimating electrical production capacity of these devices.

At the microscopic pore scale, complex redox enzymatic reactions within the pores and at the solid-fluid interface have to be described. In fact, redox mediated enzymatic catalysis process was investigated coupled to the transport of species governed by a diffusion mechanism in the bulk fluid inside the pores. In the present work, we address the case of Direct Electron Transfer for which enzyme active centers are within the tunneling distance of electron exchange surfaces. By making use of the volume averaging method [3, 4], we upscale the above mentioned microscopic problem to obtain a macroscale model. This model is characterized by a macroscopic coupled diffusion-reaction equation in the porous electrode involving an effective diffusion coefficient that can be computed from the solution of an intrinsic closure problem and from which the effective current density can be determined.

Numerical simulations are presented illustrating the capability of the multi-scale approach which provides an accurate estimation of the electrical current density with respect to the pore-space architecture providing a useful tool for electrode microstructural optimization. A successful comparison between theory and experiments is also reported.

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Nonmonotonic Pressure Field Induced by Ionic Diffusion in Charged Thin Films

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Dynamics of pressure field evolution inside thin films under the effect of ionic strength gradient is not well understood. Dynamics of the pressure field is important as it controls the film hydrodynamics and also change of contact angle due to the change of ionic strength. The major two potentials building the total pressure in thin films are osmotic and electrostatic potentials. In thin films, these two components are working against each other, while the reduction of ionic strength will decrease the osmotic pressure, it will increase the electrical double layer thickness. However, this interaction is controlled by transport of ions and the transport time-scale. Here, we present a model that couples Nernst–Planck and Poisson equations to simulate ionic transport and also Stokes equation augmented by the Maxwell stress tensor (Minisymposium T) to simulate the pressure field. Results show a highly nonlinear behavior in the pressure field that is initiated by diffusion of the ions in a channel which is initially filled by a high ionic strength electrolyte and is exposed to a bulk solution with lower ionic strength. Results show that diffusion length (transport length) and the overlapping of the double layers affect the pressure field significantly. The results imply that in thin films where ionic diffusion is expected, interfaces can deform due to the nonlinear pressure field, which is triggered by the asymmetric and multidirectional transport of ions. This brings a new insight into thin film hydrodynamics that can contribute to understanding the dimple formation in thin films.

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Simulation of porous active material in lithium ion batteries – The Newman model as an upscaling approach

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The physics inside a lithium ion battery are governed by diffusion and migration processes of lithium ions through the porous active materials. For the anode side the porous medium is graphite or hard carbon, the cathode is made from lithium metal oxides. The size of the particles is in the order of some µm, while the full electrode size is on a scale of cm to m.

In order to model the overall electrical behaviour of a full sized lithium ion battery using physical properties, most commonly the Newman model is used. The model uses an abstract representation of the porous active materials. The active material is only defined by the values for its overall porosity and tortuosity. The governing Nernst-Plank-(Poisson)-Equations are then solved on a rectangular 3 dimensional grid using effective diffusion coefficients. All equations are reformatted to obtain an equation system, which can be represented by an electric equivalent circuit. The electric equivalent circuit is used to calculate the current distributions. This approach allows a very fast and quite accurate simulation.

The effective diffusion coefficients cannot be quantified directly by measurement. Therefore they are either parameterized using fitting algorithm to obtain reasonable good match between experimental data and simulation or they are calculated by the use of further simulation tools. In this work to calculate effective diffusion coefficients the tool GeoDict from Math2Market was used. The tool is capable of importing 3D structures from 2D image slices. The 2D image slices of anode and cathode were produced using a focused ion beam scanning electron microscope (FIP-SEM).

The submitted poster will present a model to simulate the electrical behaviour of lithium ion batteries on a full battery scale and show data from the porous electrodes used to calculate effective diffusion coefficients.

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Understanding the Impedance Spectroscopy Response of Rocks – Recent Developments in Geophysics

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In Geophysics many methods exist for determining the electrical properties of the subsurface from measurements at the Earth's surface, e.g., direct current and capacitive resistivity methods, electromagnetic induction methods utilizing both natural and artificial electromagnetic sources, and ground penetrating radar (GPR). These geophysical methods cover a frequency range from mHz to GHz but each method determines the resistivity at a specific frequency only. So far, only very few studies exist which try to interpret the resistivity differences obtained by two different geophysical methods in terms of a frequency effect. On the other hand, it's known since the beginning of the last century that rocks polarize. And from the middle of the last century on, a method called induced polarization (IP), better known as impedance spectroscopy (IS) in many other fields, was applied for the exploration of conductive minerals like pyrite and graphite. Since then, IP has been applied for studying the spectral electrical behaviour of rocks in the lab and for imaging the impedance distribution in the subsurface. For the latter method, i.e. for electrical impedance tomography, instruments for time and frequency domain measurements are used. However, only frequencies well below 1 kHz can be interpreted (or even measured) with most of these instruments because impedances at higher frequencies are often obscured by electromagnetic coupling effects. Also laboratory studies on rock samples are often restricted to a frequency range up to about 10 kHz. Whereas the IP phenomenon is traditionally studied by complex resistivity/conductivity measurements, i.e. by measurements which require galvanic coupling of the electrodes, a whole bunch of research regarding dielectric spectroscopy on rocks (up to frequencies of a few GHz) has been carried out too. However, neither the combination of data studied in different but often overlapping frequency ranges nor the combination of mechanistic models addressing single polarisation processes is currently established in geophysical research. Only very recently, few studies of broadband IS measurements on rock samples as well as first attempts of combining different polarization models were published.

Nevertheless, over the last two decades significant progress has been made in understanding the microscopic mechanisms leading to rock polarization, i.e. to frequency dependent complex resistivities. Five main mechanisms have been identified in the mHz to MHz frequency range: (1) the polarization of the electrical double layer (EDL) with contributions from both its inner (Stern layer) and its outer part (diffuse layer); (2) the membrane polarization also caused by the EDL but only occurring at neighbouring narrow and wide pores; (3) the Maxwell-Wagner or interfacial polarization occurring at the solid-electrolyte interface; (4) the electrode polarization, observed in presence of conductive minerals only; and (5) high-frequency polarization mechanisms such as the orientational polarization of water dipoles.

Beside discussing the physics and the implications of these polarization mechanisms I also introduce results of petrophysical lab studies about dependencies of IS parameters on structural and electrochemical rock properties.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 514

Effect of Steam Temperature and Injection Rate on SAGD Performance

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In this paper, we try to model SAGD process physics at the grain level. The main focus is to investigate the effect of steam temperature, injection rate and wettability alternation on sweep efficiency of the process. The temperature profile and residual oil behind the steam front throughout the medium is monitored and compared to experimental information available in the literature1.

A glass micromodel structure that was experimentally tested in the literature was reconstructed, binarized and meshed using COMinisymposium OL. Then the digital 2-D micromodel was fed into OpenFOAM, which is the open source CFD package of choice in this work. The Navier Stokes equations were supplemented by different source terms, to tackle different physics. For tackling the phase change problem within the simulation, the LEE phase change model was added to the pre-defined Volume of Fluid (VOF) solver. The LEE model assumes that mass is transferred at a constant pressure and a quasi-thermo-equilibrium state. For each phase in the multi-region model, sets of mass conservation, Navier-Stokes momentum and energy equations under non-isothermal conditions are solved simultaneously.

Simulation results are in good agreement with the experiment, Figure 1. Steam chamber development and the condensation of vapor on the interface between oil and steam is observed. Viscosity reduction due to heat diffusion in the oil phase is demonstrated. Entrapment of the oil on the grains as well as temperature distribution throughout the medium is in agreement with the experiment. Imposing open flow boundaries and higher injection rates leads to fingering and smaller swept zones in comparison to zero injection rate. Changing the wettability will affect the distribution and continuity of the generated condensate.

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Effects of rock configuration and image resolution on pore-scale petrophysical characteristics

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The capability of pore-level simulations is mainly limited by computational issues related to the numerically expensive calculations. Upscaling techniques can be applied to be able to process larger volumes with less computational nodes. Here, a detailed numerical sensitivity analysis is performed to investigate the effect of rock configuration and image resolution on the effective properties of pore-level microstructures. In particular, a direct pore morphological quasi-static simulation approach is described and applied to three-dimensional images of Sandstone and Carbonate formations and partially saturated media are generated. The images are numerically upscaled covering the same domains with coarser voxel resolutions and the pore-level events are reapplied on the upscaled media. Saturation profiles are extracted and during the post-processing formation factor, absolute permeability and effective petrophysical properties, including capillary pressure and relative permeability curves, are predicted using voxel-based CFD steady-state simulations. According to the results, the effect of upscaling and resolution is pronouncedly in relation with rock configurations and pore size distributions. In general, as the resolution goes higher, small-scale pores and throats are properly captured, directly affecting the flow pathways and transport properties. However, some of the post-processing results for granular sandstones are less sensitive to the resolution within the selected range of upscaling.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 757

Permeability anisotropy determined from 3D nano-scale pore structures of organic-rich shales

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Focussed Ion Beam – Scanning Electron Microscopy (FIB-SEM) image stacks were used to reconstruct pore space and organic matter (OM) distribution in two organic-rich Posidonia Shales samples of varying thermal maturity from central Germany (WIC: R0 = 0.53 % and HAD: R0 = 1.45 %). Permeability calculations were performed on the segmented data (pixel size: 40 – 56 nm, slice thickness: 25 nm) using GeoDict and the integrated Navier-Stokes-Brinkman-LIR solver. Pores alone did not show sufficient connectivity to realize pressure drop and flux, therefore we assigned a low permeability of 1e-21 m² to the OM assuming that the OM itself contains pores below the resolution of the FIB-SEM measurements. This allowed us to build up connected porous media for permeability calculations. The results which can be found in Grathoff et al. (2016) demonstrate that absolute values of calculated permeability coefficients (k) depend strongly on the assumed OM permeability, since OM contents (WIC: 21.9 vol %, HAD: 14.7 vol %) greatly exceed the porosity values (WIC: 1.5 vol %, HAD: 2.6 vol %). However, we are able to show anisotropic coefficients for both samples, with highest k values parallel to the bedding planes which differ by up to one order of magnitude from the verticals. The observed anisotropy correlates well with values found in the literature. Additionally, our limited data indicates higher permeability for lower mature samples. Based on our data this trend may be attributed to higher OM contents that enhance pathways through the material. Since the porosity of the OM may vary with thermal maturity, we will perform ultra high resolution FIB-SEM analyses on solid bitumen particles of the two shale samples in order to improve our permeability model. We aim to present first results at the conference.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 516

Pore-Level Evaluation of Up-Scaling Techniques

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Pore-level simulation of transport phenomena has gained a lot of attention in the past three decades due to advances in imaging technologies as well as higher computational power available. It is now possible to predict petro-physical multi-phase flow properties such as porosity, permeability, formation factor, resistivity index, relative permeability, and capillary pressure using pore scale simulations. Moving to a larger scale, however, is challenging due to complex physics behind pore-scale simulators. Hence, up-scaling techniques present an alternative that should be considered and, whenever possible, be employed. The objective of this study is comparing the up-scaling techniques to extend the porous media characteristics from pore to core scale. In this research, a heterogeneous porous medium is generated using object-based modelling techniques in which the medium is generated by simulating the sedimentation process. Single phase and two phase flow properties of this medium are calculated using network modelling. Then, the medium is divided into several smaller segments and the aforementioned properties are calculated for each one of them using pore level modelling technique. Finally, several up-scaling methods are utilized to reconstruct the main heterogeneous medium using the smaller segments and calculate the flow properties using different up-scaling methods. The results are compared to the properties obtained directly from the main heterogeneous sample using network modelling approach.

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Pore-Level Petro-Physical Characterization of Shale

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To objective of this work is to investigate the multi-scale rock properties of shale matrix using digital rock physics based on actual samples of 15 nm resolution FIB-SEM images. The process of shale characterization proceeds with the accurate determination of the total and effective porosities, and the porosity associated with the Kerogen. This is followed by fast calculations of the capillary pressure curves and absolute and relative permeabilities in the X, Y, and Z directions. The process involves starting with a 2D stack of grayscale images that are manually segmented, where the different minerology associated with the shale matrix are properly identified. 3D reconstruction is then performed and the 3D image is then meshed based on voxel meshing. We then perform oil-water immiscible displacement within the pore-space using a quasi-static pore morphology approach which generates the capillary pressure curves and extracts the different saturation profiles for each phase. Using direct numerical simulations the governing equations of flow are then solved in order to generate relative permeability curves. The method leads to different saturation points for the oil and water where we observe permeability jail. Capillary pressure (assuming kerogen as a “porous plate”) generates reasonable irreducible saturations, while snap-off is the major contributing mechanism for non-wetting trapping and substantial non-wetting phase trapping is observed.

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Reasonable Use of Tight Formation Energy to Improve the Oil Production of Hydrofracture Horizontal Well

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Tight oil reservoirs are found in sedimentary impermeable formations with naturally opened or sealed micro fractures. For this type of reservoir, to achieve the economic oil production rate, the reservoir stimulation methods, especially the horizontal well and the large-scale hydrofracture, are required. Generally, a hydrofracture horizontal well starts as flowing production, and the stable flowing production can last for a certain time. In order to extend the duration of the flowing production, meanwhile t to reduce the loss of formation pressure, a reasonable production system needs to be determined. In the present work, a series of hydrofracture horizontal wells deployed for the tight oil reservoir in this depression are studied to reasonable use the formation energy. The production period of a hydrofracture horizontal well are divided into three stages, including the initial flowback stage, low pressure flowing stage, intermittent flowing stage. (1)In the initial flowback stage, the stratum energy is sufficient, and the flowing capacity is strong. Therefore, the basic strategy for reasonable use of formation energy include two aspects; primarily, the flowback velocity of the fracturing fluid should be fast; In addition, the sands flow from fractured formations should be effectively controlled. (2)In the low pressure flowing stage, the basic principles include two aspects; firstly, the oil recovery rate should be maintained relatively high; secondly, a proper difference between the flowing pressure and the saturation pressure should also be guaranteed. (3)For the intermittent flowing stage, the buildup pressure via well shut-in is the main strategy to enhance the well production. By this way, the passive intermittent flowing is replaced by the initiative intermittent flowing. The timely adjustment of the production system for different production stage to reasonable use the formation energy was proved to be beneficial for promoting the well production. This is also significant for enhancing the management of the flowing production of hydrofracture horizontal wells in a tight oil reservoir.

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Stochastic Reconstruction of Pore-level Irregular Consolidated Porous Media

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Accurate prediction of transport properties of tight and consolidated formations plays a crucial role in the development of production strategies. Permeability, thermal and electrical conductivities, pore-body and throat size distributions, relative permeability and capillary pressure curves are the most important pore-level characteristics affecting mass, thermal and electrical flows in porous media. Detailed experimental core analysis is a mature reliable tool for determining these properties in conventional hydrocarbon reservoirs. However, the inherent complexity of tight formations, as unconventional reservoirs, complicates the experimental measurement of these properties. Moreover, the designed tests for tight formation characterization are expensive, challenging and time consuming. By recent improvements in computer hardware and computational power, the simulation of transport phenomena in pore-level porous media images has become a topic of interest for a myriad of research works at academic and industrial scales. The digital rock physics modeling is improved enough to be counted as a reliable alternative for conventional techniques. Pore-scale modeling is generally divided into two main categories, pore network modeling and sub pore computational approach. Pore network modelling is applied to a network of pores and tubes with regular shapes acting as a representative model of the porous medium under consideration. The sub pore computational methods are directly applied to the digital porous media images. The governing equations of the processes are then discretized and applied to the meshed pore space geometries. In this study two different approaches are utilized to generate 3D digital porous media images based on the measured particle size distribution (PSD) data sets. For a unique real PSD, the first approach generates digital media with randomly positioned spherical grains, while the second method reconstructs packings with irregular grain shapes. As the pore structures are more realistic, the simulations at the sub-pore scale can provide more accurate predictions. An in-house software is used to directly simulate two-phase capillary-dominant displacement processes applying a quasi-static scheme. The capillary pressure curves are extracted during the simulations and two-phase transport properties are calculated by applying the governing equations to the partially saturated media. The permeability predications are then analyzed and compared with the results of the Kozeny-Carman equation. According to the results, two packings of the same PSD and porosity but different grain shapes (spherical vs irregular shape) pose dissimilar characteristics with a logical trend as the media with regular grains has lower surface to volume ratio in comparison with the media containing irregular grains.

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Voronoi tessellation-based generation of three-dimensional fractured geometry and determination of its transport properties using pore-scale simulations

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Understanding and predicting flow and transport properties of a fractured media is of key importance in various fields of human activity including oil recovery in naturally and hydraulically fractured reservoirs. Complexity of realistic fractured geometries and difficulty in assessing their geometrical features on scales relevant to macroscopic transport makes computer generation an attractive tool in studying fractured porous media. In our work, we generate a three-dimensional fractured geometry based on a simple geometrical approach and perform high-resolution flow and transport simulations in fractures, thus estimating the diffusion and dispersion coefficients as well as permeability.

We generate fractured media using Voronoi spatial tessellation. The idea behind a Voronoi tessellation is to split a target volume into simple sub-volumes without gaps and overlaps. A set of points is distributed within the target volume in an arbitrary fashion and a space region (sub-volume) closer to each point than to any of its neighbors is generated. As a consequence of this rule, each sub-volume has a polyhedral shape formed by an arbitrary number of polygons with arbitrary shapes. After determining the sub-volumes, each of them is shrunk and the released void volume is assumed to be fractures. As the porosity of this "fractured" geometry we take the ratio between the volume of "fractures" and the initial target volume.

After generating fractures, we perform discretization of the resulting geometry by introducing a fine uniform cubic mesh covering the whole target volume and assigning each voxel of a mesh as "void" or "solid" based on its spatial location, outside or inside a rock sub-volume. For this purpose we have developed a high-performance code efficiently running on thousands of CPU cores. The resulting fine mesh is used as input for single-phase flow simulations performed with the lattice-Boltzmann method. After obtaining a three-dimensional flow field, we use it to simulate advection-diffusion transport employing random-walk particle-tracking method. In this way, we can model liquid phase tracers flowing in complex fracture geometries.

In our study, we vary porosity and distribution patterns of input points resulting in different shapes and spatial orientations of "fractures" within the target volume. We can also model layered formations and formations with large fracture anisotropy. We analyze the impact of fracture geometry and connectivity on basic transport quantities such as permeability, effective diffusion and hydrodynamic dispersion.

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Aggregation-based upscaling technique for flow in fractured porous media.

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Realistic characterization of fractured porous media leads to geometrically complex models. These models are generally represented by highly detailed unstructured grids. A direct flow simulation using these large models is computationally expensive and unpractical in many situations especially when highly nonlinear flow behavior is involved. To address this problem some type of model reduction is required. In this work we focus on geometrical model reduction which is essentially the construction of a coarse grid and the evaluation of associated upscaled flow properties. In an aggregation-based upscaling technique, first a detailed fine grid model is constructed, and then the coarse control volumes are defined by grouping sets of fine grid cells. This approach is highly flexible as the shape of the coarse control volumes can easily adapt to the underlying fine heterogeneity. We use a finite volume formulation which requires a list of cells with associated volume and porosity, and a list of connections with associated transmissibility. The transmissibilities are computed using a two-point flow-based upscaling technique. The pressure field needed for the upscaling procedure is obtained by appropriately combining a set of pre-computed global fine grid pressure solutions. The same set of global pressures is used regardless of the coarse grid. This reduces the computational cost of creating new coarse models and makes the convergence study very effective. In this work we investigate different aggregation strategies. Static geological information is used to identify fractures and important matrix heterogeneity. We also use dynamic information based on flow configuration to improve the quality/resolution of the coarse grid. The methodology is illustrated with several examples.

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Dispersion in hyperporous fractured systems and the impact of matrix permeability on fracture transmissivity

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Current studies of fractures generally assume purely diffusive transport in the matrix. Yet, this assumption is invalid for fractures embedded in hyperporous matrices that can be highly permeable to flow. By means of perturbation theory and asymptotic analysis, we derive a set of upscaled equations describing mass transport in a coupled fracture-matrix system and an analytical expression relating macro-scale dispersion coefficient and matrix permeability. Our analysis shows that its impact on dispersion coefficient strongly depends on the magnitude of the Peclet number, i.e. on the interplay between diffusive and advective mass transport. Additionally, we demonstrate different scaling behaviors of the dispersion coefficient for thin or thick porous matrices. Our analysis shows the possibility of controlling the dispersion coefficient, i.e. transversal mixing, by either active (i.e. changing the operating conditions) or passive mechanisms (i.e. controlling matrix effective properties) for a given Peclet number. We compare the upscaled model against experiments conducted on microchannels with surfaces patterned with different topologies. The experimental data are in agreement with the developed theory and quantitatively confirm the impact of the matrix geometry on dispersion at different Peclet numbers. Furthermore, we demonstrate that patterned microchannels can be used as benchmarks experiments to model flows in coupled channel/fracture-matrix systems.

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Flow in unsaturated fractured porous media: Hydraulic conductivity of rough surfaces

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A percolating fracture network through a low-permeable porous media has a large effect on water flow and water redistribution. From a point of view of contaminant, both saturation degree and fluxes will influence significantly solute transport in fractured porous media. They depend on the fracture properties such as width and surface roughness. The objective of this study is to analyse how (i) properties of a fracture and fracture network influence effective properties, water fluxes and saturation degrees at the continuum scale and (ii) matrix and fracture effective properties determine water exchange and fluxes. The model of Or and Tuller (2003) is used as the basis to calculate effective flow properties of a single fracture and a distribution of fractures. Applying a model for flow under unit-gradient, the saturation degree and water fluxes both in the fracture and the matrix domains are calculated for different fracture properties (in terms of roughness), matrix properties and water fluxes. The saturation degree of fractures varies over orders of magnitude as the function of the mean fracture aperture and the fracture domain fraction as the most important parameters at high water fluxes. In a second step, a one-dimensional dual-permeability model with the fracture hydraulic conductivity model of Or and Tuller (2000) is used to analyse water exchange between fractures and matrix, equilibration time, water fluxes and saturation degrees. Water infiltration in a unsaturated fractured porous media modelled with a dual-permeability model shows a complex water infiltration and exchange behaviour.

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How estimate equivalent matrix block sizes of a fractured media from equivalent permeability tensor for dual porosity models.

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Modeling transfer in a fracture network remains a challenge. Due to the geometrical complexity of the media and to the large contrast between fracture and matrix properties, dual porosity models are commonly used. The main idea of this model is represent the flow using two media (a fracture and a matrix media). An exchange term is used to model exchange between the fracture and the matrix media. The exchange term depends on a shape factor that quantifies the mean size of the matrix block. Various formulations of the shape factor have been proposed (Kazemi et al., 1976; Thomas et al., 1983; Coats 1989; Ueda et al., 1989; Lim et al. 1995; Quintard and Whitaker, 1996; Noetinger and Estebenet., 2000). Nevertheless, it is always expansive to evaluate the mean size of the matrix blocks. A new approach was recently proposed (Jerbi et al. 2016) and succeed to derive an analytical Oriented Bloc Sizes (OBS). The main idea of the approach is that equivalent permeability tensor of a fractured media is related to the DFN skeleton and thus may help to characterize the mean matrix bloc size. Considering that a DFN may be homogenized and be modeled using a sugar box fracture model (Warren & root), analytical and oriented mean bloc sizes, si, are obtained. si depends on fracture apertures et permeabilities and associated equivalent permeability tensor. This approach was validated with geometrical considerations and on a 2 phase flow benchmark considering 3 others approaches (Bourbiaux et al 1997; Narr., 1996.; Bourbiaux et al 2006). The poster will present the different mathematical steps used to obtained the OBS model and the validation results.

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Improved Dual Porosity Modelling of Multiphase Flow Phenomena

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Fractures in geological materials are abundant. The understanding of their impact on flow dynamics is relevant for many applications. To name a few, common estimates suggest that 60 % of the remaining oil reserves are located in naturally fractured carbonates. The recovery of hydrocarbons from shales requires fracturing the rock in order to produce at economical rates. Further, the possibility of storing CO2 in fractured reservoirs and aquifers increases storage capacity substantially. On the other hand, natural or induced fractures in the caprock of a storage site might act as leakage pathways. All these applications have in common that they require an understanding of the fluid dynamics over large length and time scales while parameters are largely unknown. Therefore, a large-scale continuum approach is required, despite recent advancement in simulation technology allowing direct representation of fractures e.g. through explicitly meshing them using unstructured grids or embedding discrete fractures as additional degrees of freedom. The standard approach for large scale simulations uses multi-continuum models that treat different structures of the porous medium as separate media that exchange mass (and other conserved quantities). The upscaling challenges are 1) the identification of the separate continua and upscaling their parameters and variables and 2) the formulation of transfer functions that represent the relevant fine-scale displacement processes using large-scale multi-continuum quantities and representative geometrical and topological characteristics of the structures. Here, we focus on the formulation of transfer functions. The standard approach applies a first order transfer concept based on some potential (e.g. pressure) and simple shape factor that account for characteristic length scales. For single-phase flow in regular structured fractures (sugar cube) the solution to representative initial and boundary value problems can be expressed as a series of basis functions and hence, the conditions and regimes under which the concepts are valid is understood. This does not hold true for multi-phase flow. In particular, the early-time exchange cannot be represented as a simple first order transfer process. We use self-similar solutions, fine-scale numerical solutions and dimensionless formulations to expand and reformulate existing transfer concepts. We improve the predictive nature of transition times and shape factors. We illustrate the concepts in settings relevant for CO2 storage.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 666

Is nonlocality controlling the ergodicity of hydraulic properties in fractured formations? An analysis based on transfer functions.

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Geological heterogeneity affects the estimation of hydraulic properties of fractured aquifers. The poor characterization of the aquifer due cost-limited accessibility to the subsurface generates randomness of variables such as transmissivity (T) and storativity (S), requiring in most cases a stochastic approach to be properly analyzed. A key aspect for stochastic hydrology is to evaluate the scale of ergodicity (statistical homogenization) of the variability of T and S. A transfer-function-based model embedding a nonlocal memory function term [Russian et al. 2013] was adopted for a comprehensive examination on the implication of anomalous flow conditions on the assessment of ergodicity of hydraulic properties in a well-characterized fractured aquifer in Spain [Pedretti et al. 2016]. The analytical solution ensured a cost-effective examination of the temporal fluctuations of groundwater levels at more than 100 boreholes sparsely located in the aquifer. From the frequency of these fluctuations, the single-porosity version of the model allowed to obtain direct information regarding the spatial variability of T and S. The dual-porosity version of the model allowed to examine transmissivity and storativity of the mobile domain (Tm, Sm) and storativity of the immobile domain (Sim). We found that the type of model strongly influences the estimation of ergodicity of certain parameters, while others are insensitive to the chosen model. In particular, the use of a single- or dual-porosity domain approach does not influence the scale of homogenization of transmissivity, which is about 500m for both T and Tm. For storativities, neither S nor Sm show strong scale dependency, while Sim behaves more similarly to Tm. We conclude that care must be taken when expressing the concept of ergodicity. Indeed, ergodicity may not be universally applicable but depend on the specific effective conceptualization and model adopted for the analysis of a heterogeneous system. Moreover, ergodicity may be strictly be variable dependent.

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Solute transport in cracked concrete systems under unsaturated conditions

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The advection-dispersion transport of solutes in a cracked unsaturated concrete system is a complex process. The system is defined by a highly conductive fracture network low permeable matrix with low diffusion coefficient. The key features for solute transport in such system are the presence of the network allowing for preferential flow paths and fast solute transport, and water redistribution between the fracture and the matrix defining the water saturation degree in fractures and matrix. With this study we shed a light on the behaviour of the system under different flow and concentration boundary conditions. The conceptual model represents engineered barriers used for containment of contaminants. 2D analyses are made with an explicit representation of a complex fracture network with different percolation degrees. On the basis of the developed models we analysed the behaviour of fractured system in terms of contaminant breakthrough time and the level of retention bypass by the presence of fractures. Furthermore, we analysed the effect of fractures for different matrix transport properties. Finally the analysis on possible upscaling have been made for two types of systems, namely for boundary value problem representing the barriers through which contaminants are migrated and initial value problem representing the contamination source.

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Using topology to estimate effective fracture permeability

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In analytical upscaling of fracture permeability, fractures are usually regarded as idealized geometrical objects, scattered randomly in space, possibly with some preferential orientation. With these assumptions, the connectivity of the network is determined by the product of fracture density and mean fracture size. These are key parameters in established methods for estimating fracture permeability [1,3]. In contrast, natural fractures can branch off in many directions, and they often terminate in other fractures. The fracture size is difficult to determine unambiguously for these networks, and it is not clear whether the fracture size is predictive of the network connectivity.

In recent years, there has been an effort to apply topological concepts to characterize fracture connectivity. In the current work, we apply the node counting methodology of [2] to improve analytical estimates of upscaled fracture network permeability. We do this by replacing the fracture length by a carefully designed topological measure, which may act as a drop-in replacement of the fracture length in established permeability upscaling models. The topological parameters we use are easy to obtain from limited outcrop exposures.

To demonstrate the usefulness of the proposed topological measure, we calculate the upscaled permeability numerically for a large range of random fracture networks, both randomly scattered fractures, and networks that are based on tessellation patterns. The topological measure of connectivity is seen to unify the results to a much larger degree than the traditional measure which is based on fracture size.

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A microfluidic investigation on the impact of porous media structure on bubble fingering

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During an immiscible displacement event, there are three types of forces that govern the resulting flow regime: viscous force of the injected fluid, viscous force of the displaced fluid, and capillary force. Lenormand et al. [1] categorized the resulting flow regime when each of the forces dominate in a phase diagram, and the flow regimes are termed stable displacement, viscous fingering, and capillary fingering, respectively. In the case of gas flowing in a liquid saturated medium, the gas fingers into the medium due to the relatively low viscosity compared to the displaced liquid phase. However, Lenormand and his coworkers [1] reported that the change in the pore structure has a significant impact on the resulting flow regime during a displacement event. Additionally, Armstrong et al. [2] showed that the inertial force caused by the high interfacial velocity during a Haines jump can play a major role as one of the governing forces on the displacement, particularly when the porous medium reaches a certain pore morphological length scale. The structure of the porous medium is inevitably a major contributor to the resulting governing force and the flow regime, yet the relationship between the structural properties and the flow regime still remains unclear. Furthermore, the velocity of the interfaces can greatly vary depending on the geometry, owing to the compressibility of gas. The gas/liquid displacement in porous materials is a complex problem that requires further investigation.

Lab-on-a-chip methodologies are useful visualization tools for investigating multiphase flow behaviours in heterogeneous microstructures [3]. Bubble growth in porous materials has been visualized and investigated by employing a two-dimensional micromodel with controlled geometry [4]. Combined with high-speed imaging capabilities and simultaneous gas pressure measurement, microfluidic techniques allow an in-depth investigation of the dynamic behaviour of gas growing in a liquid-saturated porous media.

In this work, gas/liquid displacement was studied in porous micromodels with prescribed structural parameters such as the pore-throat size distribution, medium length, and porosity. The micromodel was fabricated via a soft-lithography technique. Air was injected with a range of flow rates into the micromodel and was visualized under a microscope. The gas pressure was also measured during injection and visualization. The results showed that parameters such as permeability, medium length, and porosity distribution had a significant impact on the resulting flow regime. A heterogeneous porosity led to an unpredictable behaviour of the bubble, while the change in permeability and length resulted in a clear shift in the transitional capillary number (the capillary number where fingering starts deviating from capillary fingering, indicated in Fig. 1). Also, the gas pressure at breakthrough (also known as the bubbling pressure) decreased with increasing breakthrough saturation (Fig. 1). The results provide important structural parameters that govern the resulting gas flow regime in liquid-saturated porous media.

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Adaptive Unstructured-Gridding and Fluid-Flow Property Computations on Segmented Images of Porous Media

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High-resolution 3D digital imaging has greatly advanced material science, providing the basis for the computational investigation of ensemble properties of granular porous media for continuum-scale multiphysics simulations. While such properties can be computed directly on the structured voxel grid of the digital image, alternatively, grains and pores may be represented by an unstructured adaptively refined finite-element mesh of the features of interest. The quality of this mesh strongly depends on the resolution of the original image from which the pore-grain interface is extracted as a set of surfaces. To reduce computational cost in feature-poor regions, this mesh is made much coarser than the original voxel grid. Such spatially adaptive refinement is especially attractive in media with large pore size variations.

In this work, finite-element based single phase and two-phase flow simulations are performed to evaluate the computational advantages of adaptive mesh refinement of pore types in different types of rocks. Our focus is on the computation of permeability, pore radius and capillary pressure. Pore-velocity statistics are analysed systematically in order to assess method accuracy as a function of material type and process of interest. We also present ways of automatically adapting mesh size to reduce numerical errors to obtain more precise solutions.

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An Experiment Investigation of Coal Unsteady Displacement Process

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The three-phase medium coupling relationship of coal reservoirs was consisted of coal rock, gas and water, which simultaneously determine the seepage characteristics under the multiple fields including stress, temperature and other stratum conditions. In order to study the displacement characteristics of gas-liquid two phase fluid in porous media, a custom-developed gas-liquid two-phase high precision testing system was used to carry out unsteady displacement experiment under different stresses and temperatures. The results demonstrated that the cumulative fluid production decreases with the increment of volume stress. In the range of 30℃～180℃, the measured cumulative produced liquid is the free water. Most of the liquid below 120℃ was external water, which are not sensitive to temperature changes. On the contrary, in 120℃～180℃ range, a large amount of the inner water that adsorbs on coal capillary pore was extracted and produced liquid volume grew faster than that in lower temperature range, as shown in Figure 1. Moreover, with effect of increased dynamic capillary pressure and gravity separation， the whole process of gas-liquid two-phase flow can be catalogued into three stages. The characteristics of each stage is: liquid seepage stage (stage Ⅰ) is linear, the proportion of seepage zone decreased steadily, only liquid was produced at the outlet; the gas-liquid multiphase seepage stage (stage Ⅱ), with frontier moved forward, the zone expands continuously, the gas breakthrough time shows that the mixed zone frontier has reached the end of the coal and the liquid saturation is maximum; The third stage (stage Ⅲ) is mainly based on gas flow, a small amount of liquid was driven out, forming stable single-phase gas flow gradually, but constrained liquid still exists in coal, as shown in Figure 2. In practical CBM engineering, the effect of temperature on the whole process of unsteady gas-liquid multiphase seepage is shown in the initial drainage stage, in which the drainage speed is accelerated, but the liquid production is reduced. The experimental methodology and obtained results have provided evidence in understanding the mechanisms of gas-liquid two-phase seepage and demonstrated the potential applications in CBM engineering.

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Effective Rheology of Two-phase Flow in 3D Porous Media: Experiment and Simulation

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It has been observed that, unlike the single-phase flow, the total pressure difference in two-phase flow no longer scales linearly with the volumetric flow rate in the steady state at low capillary numbers [1, 2, 3]. However most of the experimental and numerical works in this regard has been reported for 2-dimensional (2D) porous media [2] and very little work has been performed for 3-dimensional (3D) pore networks [3]. Here we present a detailed experimental and numerical study of immiscible two-phase flow in 3D porous media to find the relationship between the volumetric flow rate (Q) and the total pressure difference in the steady state. We show that in the regime where capillary forces compete with the viscous forces, the distribution of capillary barriers at the interfaces effectively creates a yield threshold, making the fluids reminiscent of a Bingham viscoplastic fluid in the porous medium, introducing a threshold pressure. In this regime, Q depends quadratically on an excess pressure drop. While increasing the flow-rate, there is a transition, beyond which the flow is Newtonian and the relationship is linear. In our experiments, we build a 3D model porous medium using a column of glass beads transporting two fluids - deionized water and air. For numerical study, we considered 3D network of pores reconstructed from real core samples [4, 5] and modeled the transport of two immiscible fluids by tracking the fluid interfaces with time. Our numerical and experimental results are in complete agreement with each other. Moreover, our results also match with the mean-field results [1] reported earlier.

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Evolution of Invading Fluids Fronts at Different Wetting Conditions

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Wettability is an important factor that controls the displacement of immiscible fluids in permeable media being relevant to many applications in oil recovery, food sciences, and the design of fuel cells. Although the influence of wettability is well captured on the continuum scale by empirical models, the quantification of wettability effects on the pore scale still poses a number of open questions. To tackle these questions, fast X-ray tomography was employed to monitor pore scale process during immiscible fluid displacement in a dense pack of beads. Applied average front velocities were in a range where capillary stresses dominate over viscous stresses on the sample scale. The contact angle of the invading fluid is varied by means of surface functionalization and using different combinations of invading and defending fluids. Two qualitatively different classes of displacement pattern were identified that are solely controlled by the contact angle. While capillary fingering controls the displacement pattern at high contact angles, the invading liquid forms a stable front at low contact angles. After injecting several pore volumes of a non-wetting invading fluid, a funicular network consisting of coalesced capillary bridges of the wetting defending fluid emerges [1,2]. The dependence of the irreducible saturation of a wetting defending fluid on the contact angle can be understood form the de-percolation of the funicular network. To quantitatively describe the displacements process in our experiments, and to facilitate a comparison with existing models, we characterize the development of the invading front by several quantities that are sensitive to different aspects of the displacement patterns. In agreement with the qualitative findings for the early stages of the displacement process, these quantities display two plateaus and a steep cross-over at neutral wettability. Variations of the residual saturations in the regime of high contact angles are a consequence of the de-percolation process that is controlled by both the contact angle and the pressure difference between the invading fluid and the defending fluid.

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Experimental investigation of two-phase flow with phase change inside porous media

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Flow boiling of natural refrigerants in horizontal tubes is a matter of considerable importance as natural refrigerants support the reduction of the carbon footprint and the ozone depletion potential of chemical plants as well as refrigeration and air conditioning systems. However, further increasing the efficiency of these apparatuses can only be achieved by simultaneously optimizing both heat transfer and pressure drop. The aim of the project presented is to verify the applicability and benefit of integrating metal sponges (open cell metal foams) in tubes for flow boiling. The highly porous network structure of sponges combined with the continuity of both of their phases allows for an improved fluid mixing and may increase the amount of nucleation sites at low pressure drops.

To date, only few researchers have investigated the heat transfer and pressure drop behavior during flow boiling in tubes filled with sponges experimentally or numerically. The contradictory results are probably due to the complex phenomenon of multi-phase flow in porous media itself, especially if combined with even more complex phase change processes. Consequently, a test section for precisely measuring the local heat transfer coefficient and pressure drop of CO2 in a horizontal tube was designed. As a result of the tube's specific design, the heat transfer coefficients at different circumferential and axial positions can be determined. Both constant temperature and constant heat flux can be set as boundary condition. Consequently, the heat transfer characteristics of different kind of sponges can be determined for a wide range of operating parameters and interpreted with respect to the observed flow pattern.

In a first step, the test section was successfully validated with both in-house data for flow boiling of CO2 and well-known correlations for heat transfer and pressure drop. Following, the flow boiling of carbon dioxide in cylindrical copper sponges with a diameter of 14 mm, a porosity of 90 % and a cell density of 10 pores per inch, which have been integrated into the test section, was characterized. In the future, the flow boiling performance is to be optimized by integrating sponges with varying properties.

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How to improve macroscopic models by pore-scale investigations?

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In the last decade, pore-scale simulations have emerged as tools offering an unprecedented opportunity to investigate physicochemical processes at the scale at which they actually occur. This has been fostered by the widespread availability of powerful computational resources and by advances in experimental techniques that allow validation and comparison with experimental observations.

Today's challenges are twofold: on one hand, there are a number of open problems related to the modeling of the physical processes and their numerical descriptions (for instance related to contact line dynamics, modeling of thin films, phase and wetting transition); on the other hand, there is an impellent need to clarify the objectives of and what can be learned to improve macroscopic model.

We primarily focus on the latter aspect, which is the most important for porous media applications, and demonstrate how pore scale simulations can be used to advance our understanding of coupled processes at the pore scale and (possibly combined into multiscale and multiphysics algorithms) to investigate how macroscopic equations emerges.

Our main objective is to discuss the opportunities offered by these tools and how they can be optimally used to improve reservoir scale predictions.

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Hydrodynamics of solute transport under two-phase flow conditions: a micromodel study

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With the use of a custom made microscope we have been able to visualize in real time two-phase solute transport in an artificial porous medium, a micro-model. The main objective of this work is to show whether clear trends for the hydro-dynamically stagnant saturation versus total saturation, as well as dispersion coefficient versus saturation, can be found using very well-controlled flow boundary conditions. A number of experiments were performed where a dispersed phase was introduced into the flow network under two-phase conditions, while the topology of the saturation was kept constant for increasing Péclet numbers. To our knowledge this is the first reported pore-scale experiment that for an identical saturation topology, immobile saturation and dispersion coefficient at different flow rates have been identified. This provides new insights into the saturation-dependency of the hydrodynamics of dispersion. For a given saturation, although the impact of flow rate on stagnant areas is not significant, its impact on dispersion coefficient is very pronounced.

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Investigation of flow velocity field evolution during ganglion mobilisation

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Immiscible two-phase flow in porous media is a process encountered in various applications such as oil recovery, soil remediation, CO2 sequestration and some other industrial systems. Almost all models of two-phase flow are based on Darcy law, which is valid only for the phases that form a continuous domain. But, there exist many applications where one of the fluid phases is (partially) discontinuous. Movement of a discontinuous phase has been the subject of various studies 1–3. There exist theories formulated on the basis of data, which analyse the phenomenon based on the overall movement of the ganglia. There is still lack of understanding of the mechanisms that lead to ganglion mobilization. One such mechanism is the interaction between the flowing wetting phase and the discontinuous phase. In this work, we focus on the interaction between the two phases and more specifically on the momentum exchange between a continuous wetting phase and a discontinuous non-wetting phase in a porous medium. As the porous medium, we used a PDMinisymposium micro-model. Two different types of fluorescent particles, with different emission wave lengths, were added to the two liquids. The two-phase flow experiment took place under a confocal microscope (Nikon A1R), which allowed us to obtain information for both phases at the same time. The acquired data were analysed with PIVlab, with which velocity fields were calculated. More specifically, we focus on the velocity field evolution within the ganglion and around it prior, during, and after the ganglion mobilization. We observed strong recirculation flow patterns within a ganglion before its mobilization. Our results shed light on the process of mobilization of the non-wetting phase ganglion due to flow of the wetting phase and the momentum exchange at the interfaces.

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Measurement of in situ contact angles in carbonate reservoir rock samples at subsurface conditions

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Wettability is the principal control on multiphase fluid distribution and flow. However, determining directly the in situ wettability, or the distribution of local contact angles, in a reservoir rock has hitherto not been possible. In this work, a micro-CT was used to image the in situ wettability distribution at the pore scale in calcite cores from a producing reservoir in the Middle East saturated with Arabian medium crude oil at subsurface conditions. A range of contact angles were measured, both less than and greater than 90o, indicating that portions of the pore space were water-wet while others were oil-wet. This mixed-wetting condition was established by a dynamic aging procedure for a period of three weeks at 10 MPa and 60oC followed by waterflooding. During ageing, the wettability was altered by adsorption of polar crude oil components, existing in the asphaltene and resin fractions, on mineral surfaces. The precipitated asphaltenes were observed with high resolution 2D scans using Scanning Electron Microscopy (SEM) and identified using Energy Dispersive X-ray (EDX) analysis. The wettability determined at the pore-scale, for the more oil-wet regions, was in agreement with contact angle measurements conducted on a pure flat calcite surface, aged for the same period of time at 60oC. However, water-wet conditions were also observed in the rock in oil-filled pores, which suggests that water in roughness of the pore space, or in adjacent micro-porosity, can protect the surface from a strong wettability alteration.

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Mechanism of Pore-scale Oil Displacement under Water-Alternating-Gas Injection

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Water-alternating-gas injection promises great potential in enhancing oil recovery as well as geological carbon sequestration. One of the main challenges in tertiary oil recovery is to recover hydrocarbons from tight microporous rock, especially from irregular dead-end pores where most oil was trapped (Figure 1). The pore-scale oil trapping mechanism is complicated under various wettability conditions and pore shapes. In order to probe the physics of oil displacement inside pores, both laser confocal imaging and lattice Boltzmann simulation method are applied in visualizing multiphase flow in rock micromodels. The micromodels are fabricated with actual rock pore-throat network patterns from micro-CT scanning. For an oil-saturated dead-end pore, the shear force applied by the water flow above the pore is unable to overcome the adhesive force between oil and pore surface (Figure 2 a). By alternating water and N2 injection, a water-N2 interface is created above the oil-wet pore, which introduces tangential capillary force to lift the oil out of the pore (Figure 2 b). Then the flow front can easily either push or drag the oil to flow away. The motion of the trapped liquid inside the pore is captured by a high-speed laser confocal microscopy. In our experiments, different pore shapes and dimensions are studied to reveal the effect of capillary force on the lifting effect. Meanwhile, lattice Boltzmann model-based numerical simulation is conducted to decouple the effects of pore surface wettability, fluid viscosity ratio, and flow rate on the oil displacement processes. Once these effects are quantified, an optimized alternating injection strategy is proposed for the whole pore network of rock micromodel. This study provides some fundamental insight of multiphase flow in microporous rock for reservoir modeling, which will ultimately contribute to enhanced oil recovery and carbon sequestration.

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Modelling of Microemulsions by Density Functional Hydrodynamics

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In this talk, we present pore-scale modeling of thermodynamic, rheological and hydrodynamic phenomena for microemulsions of Winsor I, II, and III types using Density Functional Hydrodynamics (DFH), which is the method developed by the authors during the last 20 years (Dinariev, 1995, 1998; Demianov et al., 2011, 2014; Dinariev and Evseev, 2016). The DFH provides a universal approach for multiphase compositional hydrodynamic problems. The basic assumptions of the DFH are: a) the Helmholtz energy or the entropy of the mixture is a functional depending on molar densities of the constituent chemical components, b) classical local conservation laws for components, momentum and energy are used as governing equations, c) constitutive relations and boundary conditions are consistent with the density functional. In our presentation, we briefly outline the necessary background of the DFH equations. To demonstrate consistency of the modeling, we show a set of benchmarking numerical simulations involving microemulsions and including phase equilibrium and phase transitions, rheological tests and gravitational segregation problems. We demonstrate examples of numerical simulations for industrial applications. The proposed modeling is expected to help in screening and optimization of processes used in chemical technological methods, in particular, those related to oil recovery in pores and cleaning processes.

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Modelling two-phase at pore level within the volume-of-fluid framework

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Multiphase flow in hydrocarbon reservoirs is the phenomenon that describes the movement of oil, water and gas through complex pore space of heterogeneous rock deep underground. Therefore, a pore-scale description is essential to understand the role of pore structure on the flow and transport through porous rock. We presents a simple and robust numerical scheme to model two-phase flow through porous media at the pore level. The numerical method is developed to perform multiphase direct numerical simulations at sub-pore resolution, where fluidic interfaces experience complex deformations while moving through the complicated geometry of porous media. The volume of fluid method is employed to capture the interface while its dynamic is explicitly described based on finite volume discretization of the Navier–Stokes equations. We introduce a simple yet elegant method to calculate the surface tension force from reconstructed interface elements for faces between adjacent grid-blocks that contain different fluids. Then the computed surface force is applied to the Navier-Stokes equations using a sharp formulation in such that preserves the total interface curvature. The stability and accuracy of the implemented scheme is validated on several two and three dimensional test cases.

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Multi-phase imaging of fluid rearrangement at steady state during co-injection using X-ray micro-tomography

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Dynamic flow of oil and brine in porous media is imaged at steady state by micro-CT, at a resolution of 6 µm, during the co-injection into Bentheimer sandstone. Multiphase flow in porous media is a complex phenomenon which is constituted by the interplay of capillary and viscous forces. As an important dimensionless value to evaluate the ratio of capillary to viscous forces, capillary number indicates where the viscous forces begin to dominate the capillary forces, which has a large impact on capillary trapping and remobilization [1]. Flow rate controls the capillary number through experiments, leading to different flow regimes [2]. We use micro-CT imaging to investigate pore-scale flow behaviour at steady state by systematically examining arrangements of the non-wetting phase in pore space. Two sets of experiments at high and low flow rates are provided to explore the time-evolution of the non-wetting phase clusters distribution under different flow conditions. The high flow rate is 0.5 mL/min, whose corresponding capillary number is about 10-5. The low flow rate is 0.05 mL/min, whose capillary number is about 10-6. By varying proportion of the two phases sequentially during imbibition, the pore-scale processes leading to connection and disconnection of the non-wetting phase in relation to capillary numbers are studied in detail. Four continuous images were taken at about 1 hour intervals during steady state without stopping flow were obtained and the corresponding cluster-size distributions were analysed to observe how the wetting and non-wetting phase transport at high and low capillary numbers. We provide new observations on how the capillary number impacts transition from fully connected to ganglia flow for a range of fluid saturations. We provide a detailed analysis on connected flow paths that are dominant at the low flow rate experiment, while the rate of disconnection is higher at high flow rate. Overall, we establish a workflow to experimentally characterise steady-state multiphase flow behaviour at different capillary numbers.

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NUMERICAL AND EXPERIMENTAL MODELLING OF THE FLOW FIELD IN A LABORATORY MODEL OF POROUS MEDIUM

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Numerical simulations and Laboratory experiments on porous media are an important tool for understanding the complex physics at the pore scale which is of interest for environmental and industrial processes as oil recovery, carbon storage, transport of charges in fuel cell, transport of colloidal particles in groundwater and biological flows. In these and other fields, the predictive capacity of simulations, as an alternative or complementary to experimentation, yet has to to be fully demonstrated. The objective of this work is the investigation of the pore-scale flow dynamics experimentally, through image analysis techniques and numerically, by means of computer simulations via computational fluid dynamics (CFD), using the commercial software ANSYS-Fluent. A laboratory scale real porous medium was realised employing spheres of equal size, arranged in a random packing within a square base test section. For the numerical model, an analogous porous structure was generated by means of a sequential deposition of mono-sized rigid spherical particles model. Macroscopic properties of the porous media, such as seepage velocity, tortuosity and hydrodynamic dispersion coefficient, were calculated and the connection between phenomenon observed at the macro-scale and processes going on at a smaller scale (pore-scale) established.

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Pore Scale Modeling of Enhanced Oil Recovery from Two-Phase Flow Simulations on Digital Images of Porous Rocks

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We present advances in two-phase lattice-Boltzmann simulations to increase our understanding of Enhanced Oil Recovery (EOR) mechanisms at the pore scale. Our aim is to facilitate the interpretation and evaluation of experimental results from micro-CT imaging of in-situ fluid distributions in plug samples. To achieve this goal, we develop simulation tools to capture EOR effects at the pore scale. This includes viscous forces, as the flow is no longer capillary dominated for typical surface tensions and viscosities during EOR flooding. To accomplish this, the underlying physics is captured in the numerical pore scale computations. In particular, we investigate the effects of reduced interfacial tension, viscosity alteration and large viscosity contrasts during the two-phase flow simulations. First, we optimise our proportional–integral–derivative (PID) controller for drainage and imbibition. The optimisation is validated for various systems, including a contraction-expansion and micro-model geometry. Then we apply our optimised PID controller to investigate two-phase flow in a realistic rock sample obtained from micro-CT scanning experiments. We systematically change the viscosity, interfacial tension and flow rate and observe significant differences in the dynamic saturation and saturation end points. Our simulations provide detailed predictions of the Darcy velocity, applied pressure and saturation as a function of time. Subsequently, we introduce a start-stop approach in our simulations to investigate the effect of changing the capillary number, by tuning the flow rate, viscosity and interfacial tension between the displacing and displaced fluids. We observe that the start-stop method may alter the total recovery significantly, depending on the choice of the physical parameters. In addition, we investigate the effect of viscosity contrast and observe that the rate of recovery strongly depends on the viscosity ratio. The geometries investigated include a two-dimensional micro-model of a realistic rock sample and a realistic three-dimensional micro-CT rock geometry. Our investigations provide valuable validation results for comparison with experimental results obtained from micro-CT imaging of in-situ fluid distributions in rock plug samples.

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Pore scale study of drying in porous media

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Drying in porous media is of interest to many research and engineering fields, such as recovery of volatile hydrocarbons from underground oil reservoirs, remediation of contaminant soils by vapor extraction, and water management in gas diffusion layers (GDLs) of proton exchange membrane fuel cells (PEMFCs). The drying process in a porous material is dependent on the structure and wettability of this porous material. In a porous material, the void spaces are composed of pores of various sizes. At the interface between a small and a larger pore, there exists a sudden geometrical expansion. Such sudden geometrical expansion increases the resistance to the menisci movement, and therefore is called the capillary valve effect. Because of this capillary valve effect, two types of pore invasion are revealed, i.e. bursting and merging invasion. We found that if the capillary valve effect is considered in the pore network model for drying of porous media, the modelling results will have a better agreement with the experimental data obtained from drying of a micromodel pore network [1]. For slow drying of a hydrophobic porous material where liquid flow is controlled by capillary forces and no liquid films exists, drying induced gas invasion in the porous material is a random process if bursting invasion dominates but shows a stable process when merging invasion dominates, Fig. 1. In this figure, variation of liquid distribution in a pore network during drying is shown. For drying of a hydrophilic porous material, liquid films can form in the corners of pores. We will show that the liquid films in a 2D model porous material will form capillary rings, which in turn influence the vapor transport in the porous medium. The effects of the capillary rings on the drying process will be investigated in detail.

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Probabilistic reconstruction of the 3D contact angle of two-phase fluid interfaces in porous media from a high-resolution 2D Cryo-BIB-SEM data

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It has been shown that Broad Ion Beam slope-cutting in combination with Scanning Electron Microscopy undertaken under cryogenic conditions (Cryo-BIB-SEM, Fig. 1) allows study mineral-oil-brine contacts in reservoir rocks (Schmatz et al., 2015; Schmatz et al., accepted). We studied the effect of mineralogy and fluid chemistry on the micro-nanoscale distribution of fluids in pores and measured the length of fluid-rock contact lines as well as the 2D-contact angles in slush-frozen reservoir carbonate and sandstone. All experiments were carried out under room conditions, using capillary imbibition or imbibition at low vacuum pressure, respectively, followed by Cryo-BIB-SEM investigations. Our previous work shows that the relative distribution of phases is strongly related to the mineral surface topology including surface roughness, overgrowth, mineral orientation and chemistry, next to the chemistry of the two-phase fluid. We used dedicated image analysis software, which can be used for phase segmentation based on SE, BSE and EDS data. The segmented data-set was analyzed and in the mixed-wet cases, we determined more than 2000 contact angles in typical Cryo-BIB-SEM 2D data sets of around 0.5 mm2, which were measured and analyzed with respect to the minerology and the mineral surface topology (Fig. 2). However, the BIB-cut cross sections are 2 dimensional and can hence only be used to assess the apparent contact angle, which is influenced by the orientation of the mineral surface towards the cross-section. In theory the distribution of the measured apparent angle is related to the distribution of the 3D angle. We aim a reconstructing the 3D contact angle from the 2D data. In this contribution we present a geometrical model that explains how a single 3D angle results in a distribution of 2D angle. Next we compare the results of the probabilistic model with the experimental results for different mineral surfaces (Quartz, Kaolinite and Calcite) and different surface topologies (planar vs. curved, smooth vs. rough) to i. discuss the applicability of the model and ii. to define the main influencing parameters on the development of the microscopic contact angle und given experimental conditions.

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Quantitative Investigation on Pore-scale Displacement of Porewater by Supercritical CO2 Injection Using a 2D Micromodel

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Geological CO2 sequestration is one of the most important technologies to mitigate greenhouse gas emission into the atmosphere by isolating great volumes of CO2 in deep geological formations. This novel storage option for CO2 involves injecting supercritical CO2 into porous formations saturated with pore fluid such as brine and initiates CO2 flooding with immiscible displacement. In this study, a 2D porous micromodel was applied to estimate the effects of geological conditions and injection methods on displacement of resident porewater by injecting scCO2 in the pore scale. Binary images from image analysis were used to distinguish scCO2-filled-pores from other pore structure. CO2 flooding followed by porewater displacement, fingering migration, preferential flow and bypassing were observed during scCO2 injection experiments. Effects of pressure, temperature, salinity, flow rate, and injection methods on storage efficiency in micromodels were represented and examined in terms of areal displacement efficiency. The measurements revealed that the areal displacement efficiency at equilibrium decreases as the salinity increases, whereas it increases as the pressure and temperature increases. It may result from that the overburden pressure and porewater salinity can affect the CO2 solubility in water and the hydrophilicity of silica surfaces, while the neighboring temperature has a significant effect on viscosity of scCO2. Increased flow rate could create more preferential flow paths and decrease the areal displacement efficiency. Compared to the continuous injection of scCO2, the pulse-type injection reduced the probability for occurrence of fingering, subsequently preferential flow paths, and recorded higher areal displacement efficiency.

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Sherwood Number Correlations for Pooled NAPL dissolution in Porous Media

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Interphase mass transfer is the governing process in the dissolution of non-aqueous phase liquids (NAPLs) entrapped in porous media. Dissolution from a unit surface area of NAPL into the adjacent mobile aqueous phase is commonly modeled at the continuum scale as the product of a chemical potential and an interphase mass transfer coefficient, the latter expressed in terms of Sherwood number correlations that are related to flow and porous media properties. Because of the lack of precise estimates of the interface area separating the NAPL and aqueous phase, numerous studies have lumped the interfacial area into the interphase mass transfer coefficient. To date only two studies with non-lumped Sherwood correlations can be found in the literature. In this paper controlled dissolution experiments from pooled NAPL were conducted. The immobile NAPL mass is placed at the bottom of a flow cell filled with porous media with water flowing on top. Effluent aqueous phase concentrations were measured for a wide range of aqueous phase velocities and for various porous media. To interpret the experimental results, a two-dimensional pore network model of the NAPL dissolution was developed. The well-defined geometry of the NAPL-water interface and the observed effluent concentrations were used to compute best-fit mass transfer coefficients and non-lumped Sherwood correlations. Comparing the concentrations predicted with the pore network model to simple previously used one-dimensional analytic solutions indicates that the analytic model which ignores the transverse dispersion can lead to over-estimation of the resultant mass transfer coefficient and the Sherwood. The predicted Sherwood correlations are also compared to previously published data and implications on NAPL dissolution rates are discussed.

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Stochastic Rotation Dynamics simulations of wetting multi-phase flows in porous media

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Wettability is a key factor that governs how a fluid is displaced from a porous solid by another immiscible fluid. Numerical simulations of these multi-phase flows at partial wetting conditions are still challenging as they invariably involve moving fluid-fluid interfaces in contact to the surface of the solid. With the aim to study the effects of wettability on interfacial flows on the pore scale, we developed an extension of Inoue's particle-based simulation approach for immiscible fluids [1] that allows us to continuously vary the equilibrium contact angle with the pore walls. In this variant of the stochastic rotation dynamics method, immiscibility of the fluid phases is achieved through a collision operator that actively separates fluid particles of different colors. Variations in the relative adhesion of the fluids to the solid are realized by assigning colors also to virtual particles that ensure a proper no-slip boundary condition at the walls [2]. This renders our multi-color SRD approach particularly suited to consider wetting flows with topological changes of the fluid-fluid interfaces, as encountered during the pinch-off or the coalescence of droplets. To validate the multi-color SRD method, we compare the entry pressure for throats formed by three spherical beads to corresponding results of numerical energy minimizations. Simulations of slow fluid displacement from quasi-two dimensional arrays of cylindrical obstacles [3] and in random packs of beads [4] show a good quantitative agreement with experiments.

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Study of wetting behavior from low to high capillary numbers: A new model for liquid-solid interactions on the pore-scale

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The description of wetting phenomena on the continuum scale is a challenging problem, since intermolecular interactions like the Van der Waals forces between liquid and solid alter the flow-field at the contact line. Therefore, we present SPH simulations on the continuum scale using the physically based Contact-Line-Force model in a wide range of wetting dynamics and compare them with experiments of forced wetting. For the presented cases, it is shown that at high wetting speeds the CLF-model reaches dynamic contact angles in close range with the experiments. However, at low wetting speeds the experiments show that most of the driving-force is dissipated to overcome strong liquid-solid interactions. Therefore the existing CLF-model is extended to capture those liquid-solid interactions in the stick-slip regime of wetting-dynamics.

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Two-phase flow through thin porous layers: beyond extended Darcy's law

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Two-phase flow through thin porous layers is encountered in a number of industrial applications. For instance, it plays a crucial role in the water management of polymer electrolyte fuel cells (PEFCs). Over the past two decades, at the macro scale, air-water flow through diffusion layers has been overwhelmingly modeled with the extended Darcy's law (i.e. two-phase Darcy's law). However, evidences have shown that it fails in predicting the water flooding in thin diffusion layers of a PEFC. According to our knowledge, there are two primary reasons for the failure. One is due to the failure of the conventional REV concept in the gas diffusion layer (GDL), which has been explained in detail in (C. Z. Qin & Hassanizadeh, 2014). Meanwhile, a new model called the reduced continua model (RCM) has been developed (C. Z. Qin & Hassanizadeh, 2015). The other reason for the failure is due to that liquid water transport in diffusion layers is under an extremely small capillary number (

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A Bayesian assessment of an analytical model for steady-state flow in multi-layered porous media with applications to railway track drainage

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The modelling of water flow in multi-layered porous media is still a challenging problem with profound implications to safety and cost in several engineering applications. Such is the case for railway track drainage, which, in most current railway tracks, mainly relies on natural infiltration of water through several layers with different hydraulic conductivities. The retention of water within the track substructure is known to be a root cause of several track problems, such as settlements, poor geometry, and accelerated track ageing. Track drainage is generally given insufficient attention during design and service, perhaps because of the lack of practical but rigorous modelling tools for practitioners and maintenance engineers, along with the complexity of available computational models for accurate system predictions, like finite element or finite differences models. In this paper, an analytical model for steady-state water flow in multi-layered porous media is proposed based on a Dupuit-Forcheheimer analysis [1]. The proposed model predicts the steady-state water table elevation for a multi-layered sloping system with recharge (rainfall). The key contribution in relation to a similar model from the literature [2] relies on the ability of the proposed model to consider more than two layers with different thicknesses and slopes, so that the approach in [1] becomes a special case of the proposed model. Such a generalization for more than two layers is crucial when long-term track service conditions are taken into consideration (e.g. additional layers due to fouling, ballast tamping, etc.). In addition, a novel Bayesian model testing method is proposed whereby the performance of the model is assessed through probabilities that measure the extent of agreement of the proposed model against a reference finite-difference model using MODFLOW [3]. A Markov Chain Monte Carlo algorithm is adopted to solve the resulting Bayesian inverse problem. Results show the suitability and predictive accuracy of the proposed model against the reference MODFLOW model.

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A stochastic micromechanical framework for porous media

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A stochastic micromechanical framework is proposed to characterize the probabilistic behaviors of the effective properties of porous media. The deterministic micromechanical model is utilized to quantitatively relate the material's microstructures and macroscopic properties. By modeling the volume fractions and properties of constituents as stochastic, we extend the deterministic framework to stochastic to incorporate the inherent randomness of effective properties among different specimens. A distribution-free method is employed to get the unbiased probability density function based on the maximum entropy principle. Numerical examples including limited experimental validations, comparisons with existing micromechanical models and the Monte Carlo simulations indicate that the proposed models provide an accurate and computationally efficient framework in characterizing the effective properties of porous media.

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An Optimal Balancing Strategy for Sampling and Discretization Errors in Multi-Level Monte Carlo

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Statistical means computed by Multilevel Monte Carlo (MLMC) are subject to two types of errors, that is a sampling and a discretization error. While we can influence the discretization error by changing the grid hierarchy that comprises the different levels in an MLMC computation, the sampling error can be controlled by adjusting the numbers of samples invested at the different levels. In this work [1], we present a strategy for balancing the two errors that guarantees optimality. Other suboptimal balancing schemes may achieve the same sampling error but at possibly larger computational expenses. We illustrate our new approach by calculating the mean water saturation in a two-phase flow and transport application in the heterogeneous porous subsurface.

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Analysis of travel time distributions for uncertainty propagation in realistic heterogeneous porous systems

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Reservoir simulation with realistic porous systems involve large-scale and complex porous media, coupled with incomplete geological information due to scarce and expensive data acquisition processes. Yet, reservoir simulation aims at predicting the state of the oil production at wells by, for example, providing the saturation fields at any given moment of the simulation. The uncertain geological properties of the reservoir encourages a stochastic treatment of the saturation fields, and we choose to focus on the evolution of the saturation probability density functions (PDF). According to [1], estimating the saturation PDF can be efficiently achieved by first considering the PDF of the travel time, the time it takes for a particle to travel from an injector to a specified position. Hence, the study of the travel time PDF is the main topic of this work. Indeed, geological realism is an increasingly important aspect of the uncertainty assessment in reservoir simulation. Geological properties usually have multi-scale and heterogeneous character, which is difficult to describe analytically. Most of the uncertainty quantification approaches assume some kind of stationarity for the input random models (for example, it is common to assume that the permeability field is a log-Gaussian field with exponential covariance). However, we investigate the properties of the travel time PDF when the underlying heterogeneous permeability field is captured using multi-point geostatistics [2], in particular channelized systems obtained from training images. We show that there are interesting spatial transitions in the travel time PDF behaviors, and explore the effects of conditional vs unconditional, as well as binary vs bimodal permeability realizations on the travel time statistics. We believe that with the known distribution of the travel time for these complex input fields one could efficiently incorporate them in the distribution method framework [1] and thus provide a reliable estimate of the saturation uncertainty.

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COMBINED EFFECT OF PIEZO-VISCOUS DEPENDENCY AND SURFACE ROUGHNESS ON COUPLE STRESS POROUS SQUEEZE-FILM CIRCULAR PLATE

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The theoretical study of the effects of pressure dependent-viscosity and surface roughness on the squeeze film lubrication between circular plates is presented in this paper. On the basis of Christensen's stochastic theory for rough surfaces the modified averaged Reynolds equation is derived. The closed form expressions are obtained for the mean squeeze film pressure, load carrying capacity and squeeze film time. The results are presented for different operating parameters. It is observed that, the effect of azimuthal (radial) roughness pattern on the bearing surface is to increase (decrease) the mean pressure, mean load carrying capacity and squeeze film time and the effect of permeability is to decrease the pressure, load carrying capacity and squeeze film time.

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EFFECT SLIP ON A VISCOUS FLOW OVER A SHRINKING SHEET WITH MASS TRANSFER IN POROUS MEDIUM

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In this note, we investigate effect of Navier's slip viscous flow over a shrinking sheet with mass transfer in a porous medium is considered. This problem is mapped into nonlinear ordinary differential equations by a similarity transformation. The highly nonlinear equation is solved analytically. Newtonian fluid is extended to include porosity effects, slip and wall mass. The effects of various parameters such as porous, Navier's slip and viscosity parameter, on velocity profiles are presented and discussed. The present study throws light on the analytical solution of a class of laminar boundary layer equations arising in the shrinking sheet problem.

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EFFECTS SLIP ON A VISCOUS FLOW OVER A SHRINKING SHEET WITH MASS TRANSFER IN POROUS MEDIUM

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Gaussian Process Modelling for uncertainty quantification in fluid flow in porous media

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In this paper we develop field emulators for a finite element porous media flow field simulator with a random permeability field. We predict the velocity and pressure fields with high resolution, from which scalar summaries of the output can be extracted using quadrature rules.

The challenges fall into two categories: the high dimensionality of the input space (describing the permeability field) and the high dimensionality of the output space (pressure/velocity values at the FE nodes assuming a nodal basis). Two approaches are taken: a data-driven approach based on Gaussian processes and a Galerkin finite element reduced order model.

For the first we employ a KL expansion for the input and manifold learning to reduce the dimension of the output space, that is we locate a manifold on which the high dimensional outputs (vectorised pressure/velocity values at the FE nodes) reside and find an inverse map from the reduced dimensional coordinates to the physical space.

In a second approach we employ a KL expansion for the input space and use proper orthogonal decomposition to reduce the output space dimension. The snapshots for new input values are learned using high-dimensional output emulation based on manifold learning, as described above. This the approach is ideal for uncertainty quantification. We also investigate the use of generalised polynomial chaos expansions as an alternative to KL decomposition.

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Influence of flow characteristics on rainfall-triggered instability of heterogeneous unsaturated slope

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Transport of water flow in heterogeneous unsaturated soils is intrinsically complex and depends strongly on the flow characteristics. Understanding the governing factors that influence these characteristics is useful for various applications related to transport in multiphase porous media. In particular, this knowledge is critical for investigating unsaturated slope instability triggered by rainfall in geotechnical engineering. Infiltrated rainfall into a porous unsaturated soils can lead to suction reduction and, possibly, positive pore pressure rise. Both these effects directly contribute to reduce soil shear strength and, hence, destabilise the slope. If the soil porosity significantly varies in space, an extra level of complexity is added because water follows preferential paths causing uneven reduction of suction over the domain (Le et al, 2012). This study investigates the influence of the flow characteristics on the stability of an unsaturated slope with spatially varying porosity subjected to a rainfall event (Fig. 1). The study examines the effects of initial water table depth, rainfall intensity, permeability and water retention characteristics. The random finite element method and the shear strength reduction technique (Griffiths & Fenton, 2004) are employed to estimate the factor of safety of the slope and the size of the sliding mass during and after the rainfall. The results show that the interaction between porosity heterogeneity and partial saturation can lead to complex patterns of variation over time of both the factor of safety and the size of failure mass. Heterogeneity of porosity can alter the failure mechanism during rainfall (Fig. 2). Increase in rainfall intensity leads to a faster and greater drop in suction, and consequently elevates the risk of failure. Whereas, the effect of increasing saturated permeability is rather unexpected. The intermediately permeable soils pose the highest risk of unsaturated slope failure triggered by rainfall (Fig. 3). The high permeability allows the pore water pressure to dissipate quickly while low permeability impedes the flow; both of these effects decrease the risk of failure induced by infiltration. The initial hydrological condition of the soil mass also plays an important role as reflected by the influence of water table depth. Dry soil with low initial water table increases the slope stability during rainfall because of extra shear strength provided by large soil suction. The trend is opposite for wet soil with high initial water table. The variation of the parameters controlling the dependency of water retention behaviour on porosity and the gradient of the water retention curve are also considered. Unsaturated flow preferably migrates through high porosity soil elements if there is no dependency of the of the water retention curve on porosity but switches to preferring low porosity element if this dependency becomes more pronounced. The risk of failure is shown to be significantly lower if there is no dependency of the water retention curve on porosity. The effect of the gradient of the water retention curve is rather non-linear and non-monotonic due to the simultaneous influence in both the degree of saturation and relative permeability. Overall, the risk of failure is higher for small to intermediate than for large values of this gradient due to the higher initial degree of saturation.

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NANOFLUID FLOW OVER A SUPER-LINEAR STRETCHING SHEET IN POROUS MEDIA

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In this paper, we investigate the flow due to a super-linear stretching sheet in porous media. We discuss the analysis of a mathematical model describing the nanofluid due to a perforated sheet undergoing super-linear stretching sheet in a fluid at rest is a process in which the ambient nanofluid in the presence of porous media and suction/injection are taken into consideration. The governing system of partial differential equations describing the problem is converted into a system of non-linear ordinary differential equations by using the similarity transformations. Three types nanofluids, namely Copper (Cu), alumina (Al2O3) and Titania (TiO2) are considered in water as the base fluid. An analytical form was presented by Crane for the steady boundary layer flow of an incompressible Newtonian fluid, which was solely caused by the stretching of an elastic flat sheet. The axis is chosen perpendicular to the stretching sheet and the sheet was stretched horizontally by pulling on both ends with equal forces parallel to the sheet (in the absence of body force and an external present gradient) with a speed , which varied linearly with the distance from the slit. It is shown that the behavior of the fluid flow changes with the change of the nanoparticles type. The study of the nanofluid due to a perforated sheet undergoing super-linear stretching sheet in a fluid at rest is an important aspect of various industrial applications. For instance, in polymer extrusion processes, the extruded material passes between two solid blocks into a region containing fluid at rest that cools the sheet and alters its mechanical properties.

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NEWTONIAN FLUID FLOW PAST A PERMEABLE STRETCHING/SHRINKING SHEET IN A POROUS MEDIUM

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In this talk, Newtonian fluid flow past a permeable stretching/shrinking sheet embedded in a porous medium using a proposed Brinkman model. The governing system of nonlinear partial differential equations describing the problem is converted to a system of non-linear ordinary differential equations by using the similarity transformations. Analytical solution is obtained for velocity. The effects of the Brinkman number or viscosity ratio, slip parameter, Darcy number, suction/injection parameter and the mass suction parameter on the velocity distribution are presented graphically and discussed. The results have possible technological applications in extrusion process and such other allied areas and in the fluid based systems involving stretchable materials.

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Non-Darcy inertial fluid flow in heterogeneous porous media

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We investigate local aspects and heterogeneities of porous medium morphology on the inertial flow, and relate them to the relevant mechanisms of momentum transfer. In the inertial range, there are very few experimental data that allow to recognise the effects of porous structure on the flow and transport through porous media. An experimental analysis was performed in order to understand above processes at different Reynolds numbers in regularly and randomly structured porous media. The objective of the analysis is to explore the effects of randomness in the morphological structure of porous media on inertial and viscous forces and determine range of the Reynolds numbers in which the inertial flow predominantly contributes in dispersive processes. Transport characteristics of the randomly structured porous media and the influence of inertial force on longitudinal and transverse dispersion coefficients were studied. In addition to the experimental analysis, a three-dimensional computational framework was developed and numerical simulations were performed for the flow and transport problems in order to model the deviations from Darcy's law observed in the experiments. The framework is capable to capture a gradual transition from linear to nonlinear flow regimes and reflect the influence of the flow field on the transport mechanisms. We statistically characterize the random structure of porous medium in terms of random realizations of porosity and permeability fields. This allows us to interpret certain features of the fluid flow and transport phenomena in heterogeneous porous media that have not been studied before. As the hydrodynamic dispersion is a function of the fluctuations of the fluid flow field [1 and 2],a strong connection is observed between the structure of porous domains and dispersion transport process. The results of our simulations agree with numerous experimental data which display significant increase in transverse dispersivity when the Reynolds number increases.

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Numerical modelling of rainfall infiltration in partially saturated soil within railway track system

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Rainfall infiltration plays an important role in the long term performance and overall safety of railway infrastructure. Although the significance of an adequate level of ballast drainage capacity is widely recognized, the role of subgrade characteristics in drainage performance of the railway infrastructure is neglected to a large extent. This is especially important since the subgrade layer is designed to be within the partially saturated zone, while the rainfall infiltration can lead to a change in pore water pressure regime from negative to positive. Rainfall-induced accumulation of water within the track substructure reduces the shear strength and bearing capacity of the subgrade layer and may lead to track failure or fines being 'pumped' into the ballast due to train loading. Given that changes in rainfall patterns and its spatial and temporal variabilities are expected as a result of climate change, re-evaluation of drainage capability of railway track systems is required. The inherent uncertainty of rainfall patterns can be better captured using intensity-duration-frequency (IDF) curves, which are essentially a statistical representation of the variation in rainfall intensity and duration for a given return period. Therefore, the IDF curves of the UK have been derived in order to establish realistic precipitation variations and the likelihood of intense rainfall and/or rainstorm events. Then, the rainfalls are implemented in a finite element numerical model developed in ABAQUS. The model employs a partially saturated flow scheme using Darcy's law and Richard's equation. The suction (i.e. capillary pressure) is estimated using Van Genuchten's water retention curve, which contributes to pore pressure variations and shear strength alterations within the railway track system. A parametric study is conducted to investigate the effect of subgrade properties and hydraulic boundary conditions on the resilience of the railway track system to the simulated variations of rainfall intensity and duration.

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Stochastic analysis of rainfall-induced instability in mining spoil dumps with variably distributed soil-water characteristics

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Lignite mining requires excavation of large amounts of overburden materials, also known as spoils, which are deposited in internal or external heaps. Spoil materials are a special case of anthropogenic soils whose physical and engineering properties are largely variable, both spatially and temporally. The stability of dumps is imperative in order to ensure safe mining operations and post-mining reclamation processes. Review of the reported instabilities in spoil dumps of European lignite mines revealed that almost all are induced by rainfall (see Bednarczyk, 2016; Steiakakis et al., 2009). Existing studies on rainfall-induced slope instability are mainly concentrated on homogenous soils while those concerned with variably distributed soil properties are usually limited to the case where cross correlations between soil properties are considered but the spatial variability is neglected. However, owing to the deposition methodology of spoil materials, a random distribution of properties seems more appropriate to better capture the uncertainty related to water flow in slopes and induced instabilities. Recently, few studies have employed stochastic analyses to study rainfall-induced instability in which randomly distributed soil properties have been utilised (e.g. Songa and Borja, 2014; Le et al. 2015). However, there are some shortcomings with the existing studies on random soil properties. First, these studies are mostly concerned with safety factor and hence, limit analyses have been used to determine the likelihood of instability in slopes, and therefore, improved coupled hydro-elasto-plastic models are needed to enhance the prediction of instabilities and the understanding of their mechanisms. Second, the significance of randomly varied parameters of soil-water characteristic curve have not been examined in the literature which this needs be addressed. In order to achieve these, a coupled hydro-mechanical model is developed in ABAQUS, where the unsaturated flow is described by Darcy's law, formulated in Richard's equation. Moreover, the effect of negative pore pressure on shear strength of unsaturated soil is explained by the Bishop's definition of effective stress, while Mohr Coulomb failure criterion is used in conjunction with a non-associated flow rule to model the plastic deformation within soil. The soil-water characteristic curve is represented by van Genuchten equation. Data from Turow lignite mine spoils are used to estimate Probability Density Function (PDF) for unsaturated soil properties. A Monte Carlo simulation is then conducted where each of the randomly-generated distributions of soil properties are analysed within the coupled hydro-mechanical model to assess the rainfall infiltration and the induced instabilities. The size of the sliding mass is presented, as well as pore water pressure and deformations at sampling points to discuss the mechanisms of rainfall-induced instabilities in slopes with randomly variable properties.

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THERMOSOLUTAL MARANGONI BOUNDARY LAYER FLOW VISCOUS FLUID OVER A POROUS MEDIUM

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The present paper of thermal diffusion and diffusion thermo effects on thermosolutal Marangoni convection flow in the presence of embedded in a porous medium is considered in the laminar boundary layer approximation. The governing system of partial differential equation is transformed to a set of nonlinear ordinary differential equations, Using appropriate similarity transformations is solved by applying Adomian decomposition method (ADM), differential transform method (DTM) and Pade approximants. The exact analytical solution could be obtained in terms power series which takes rapid convergence and each terms are easily computable. The effects heat and mass transfer characteristics of the flow as functions of the physical parameters namely Darcy number, heat generation coefficient and the chemical reaction coefficient on the velocity, temperature and concentration profiles as well as the wall velocity are presented and discussed.

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Uncertainty evaluation in modelling of matrix acidizing process: Effects of rock heterogeneity and porosity/permeability feedback from geochemistry

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Matrix acidizing is the process of dissolution of the sediments, mud solids and minerals within the pores of siliciclastic or carbonate hydrocarbon reservoirs that are inhibiting permeability of the rock, thereby enhancing the injectivity and productivity of hydrocarbon recovery operations. The process features a strongly coupled flow and geochemistry, where the physical properties of rock such as porosity and permeability dynamically evolve across multiple time and length scales. From operational point of view, it has been shown that there is an optimal rate of acid injection under which the breakthrough of acid on core samples can take place with a minimum pore volume injected [1]. In other words, the least amount of acid is required to generate or recover the intended and desirable flow pathways (wormholes for carbonates) by geochemical dissolution. This has been shown to be controlled by the the rock lithological properties (permeability) and mineralogical heterogeneity [2,3]. We develop a numerical modelling of core-scale acidizing operation, and validate the numerical tool against a series of experimental data for acidizing carbonate and sedimentary cores. We conduct the simulations in presence of varying spatial degrees of lithological and mineralogical heterogeneity and we consider different relationships for the porosity/permeability feedback from geochemical reactions. The accuracy of existing constitutive relationships for the evolution in porosity-permeability due to the acid-induced geochemical variations of the porous systems will be further discussed. We also investigate upscaling of such processes and the effectiveness of upscaled resolutions to replicate the optimality curve.

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Uncertainty of suction measurement with tensiometers

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Climate change and environmental variations can significantly influence the pore-water pressure and shear strength of the shallow depth unsaturated soils. Small variations of negative pore-water pressure (suction) during wetting and drying cycles can cause slope failures and landslides. This highlights the importance of accurate and continuous observation and measurement of soil suction during wet and dry seasons. Among the available direct suction measurement methods, tensiometer is the most reliable method for laboratory and in-situ measurement. Recently, high-capacity tensiometers (HCTs) have been developed for measurement of soil suction up to 2 MPa. HCTs have received significant interest in laboratory testing of unsaturated geomaterials mainly due to their fast response time, and ease of transport and installation in geotechnical apparatuses. However, despite various design and experimental procedures adopted to improve the HCTs' performance, uncertainties and inconsistencies still exist with regards their measurement accuracy, range and duration, the latter being a function of cavitation occurrence before pressure equalization. In this work, an experimental program is adopted to address these uncertainties. Several prototypes of an in-house designed HCT are constructed. Novel techniques are employed to minimize the potential of cavitation occurrence during suction measurements, hence, improving the measurements range and duration. These prototypes are tested under similar controlled testing conditions with the aim to evaluate the factors causing identical tensiometers having inconsistent measurements. The obtained results are further compared with the results of an indirect suction measurement technique, namely filter paper, carried out under the same testing conditions. It is found that, for the adopted design and experimental procedure, a relative tolerance range in suction measurements is quantifiable and can be implemented in practical design and analysis.

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Uncertainty Quantification for Flow in Heterogeneous Media with Sparse Polynomial Chaos Expansion constructed by Feature Selection

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In this study, we explore an efficient stochastic approach for uncertainty analysis of flow in heterogeneous media, where a sparse polynomial chaos expansion (PCE) response surface is constructed with the aid of feature selection method. With the PCE method, the random structure of flow field can be efficiently characterized by some polynomial chaos functions and the uncertainty quantification is equivalent to evaluating PCE coefficients. However, the number of basis function grows exponentially with the random dimensionality increasing, which makes the computational cost unaffordable to simulate adequate realizations for high-dimensional problems. To address this “curse of dimension” problem, the feature selection method is introduced in this study to select those significant stochastic features. In this setting, a reduced number of basis functions is retained and a sparse PCE response surface can be constructed with less computational effort. Inspired by statistical learning theory, the selection task is accomplished by the least absolute shrinkage and selection operator based on least angle regression (LASSO-LAR). The cross-validation (CV) method is applied for assessment and inherited samples are utilized to make the algorithm self-adaptive. In this study, the sparse PCE method in terms of accuracy, efficiency and applicability for flow in heterogeneous media with different spatial variability and flow type is mainly discussed. The numerical experiments indicate that the sparse PCE approach is able to accurately estimate the statistical moments and probability density function of the output random field, meanwhile the computational efforts are greatly reduced compared to the Monte Carlo method.

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Upscaling particle dispersion and reaction in random flow fields

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Real-world complex flows are typically characterised by the existence of multiple length scales and, despite the many computational and theoretical advances in Direct Numerical Simulation and Multi Scale numerical methods, their simulation still rely often on empirical or semi-empirical effective correlation, to explain and simulate the emerging macroscopic dynamics. We review here some modelling challenges related to the upscaling of (possibly anomalous) dispersion and adsorption of colloidal particles in flow fields generated by random porous media or steady turbulence-like flows. Different upscaling techniques are considered, including mathematical homogenisation, Lagrangian coarse-graining, volume averaging and the PDF approach.

Macroscopic model derivation and three-dimensional numerical simulations are presented for two examples of such flows: first, an extended thermodynamics coarse graining is performed on Lagrangian passive particle transport, including inertia. In the second example, particles undergoing fast reaction and/or adsorption in complex porous structures are studied via two-scale asymptotics.

These two examples illustrate the relations and complementarity of the upscaling approaches, and the need of rigorous, yet practical, multi-scale methodologies for enabling predictive macroscopic simulations.

Finally, a practical computational approach is proposed to approximate the closure problems in a random setting via Multilevel Monte Carlo sampling. Applications to subsurface hydrology and rechargeable batteries will be presented.

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An Analytical Method for Analyzing Performance of Multiple-fractured Horizontal Well in Tight Oil Reservoirs

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Inflow performance relationship (IPR) describes the relationship between a well's inflow rate and flowing pressure, it plays an important role in nodal systems analysis and productivity prediction. The steady flow is usually assumed on traditional IPR curves, not as a function of time. However, tight oil reservoirs may take several years to reach stabilization due to the extremely low permeability. As a result, traditional IPR curves are not applicable for such unconventional reservoirs. Multiple-fracture horizontal wells (MFHWs) have become the most effective technology for exploiting in tight oil reservoirs. Accordingly, a semi-analytical flow model of MFHWs based on trilinear flow and superposition principle is established in this paper. The approach can be used to generate the IPR curves with consideration of production history under production rules of constant flowing pressure, constant production rate, intermittent production, or even more complex cases. This paper discusses the differences between conventional IPR curves and transient IPR curves. Furthermore, the effect of production history on transient IPR is investigated. Finally, the example of field data is matched and the transient IPR curve is plotted to support the approach in this paper. A remarkable advantage of the proposed method is that the new model is no longer limited by constant flowing pressure or production rate conditions in comparison to the previous analytical model, so the transient IPR curves can be generated based on production history matching. On the traditional IPR curve, the intercept is the average reservoir pressure, however, the transient IPR intercept is not representative of the average reservoir pressure but equals the well pressure if the well were shut-in for that duration, and the curves are affected by the production history. The methodology and results presented in this paper are practical, and can be used directly for production forecasting and nodal analysis of MFHWs in tight oil reservoirs.

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Effects of cleat geometry of coal on permeability evolution: a pore-scale network modeling approach

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Permeability of coal exerts profound effects on both primary coalbed methane (CBM) productions and CO2 injectivity and sequestration in underground CBM reservoirs. During these processes, the permeability of coal exhibits complex dynamic behaviors with varying gas pressures due to the opposing effects of matrix shrinkage (swelling) and pore pressure decrease (increase). Although a variety of analytical models have been proposed for simulating the evolution dynamics of coal permeability, a majority of these models assume a homogeneous nature of the coal cleat system (e.g., match-stick and cubic models), which in reality can hardly be satisfied. This paper proposed a framework that integrates pore-scale network modeling with rock geomechanics analysis to model the coal permeability dynamics. Hagen-Poiseuille's equation combined with cleat deformation quantification were coupled to capture the evolutionary trend of coal permeability. The proposed model relaxes the prior assumption of a homogeneous and/or isotropic nature of coals and provides with a new solution for interpreting coal permeability dynamics from cleat geometries. The validity of the model was tested against experimental data acquired from previous studies, which showed a close agreement between the modeled and measured permeability evolution profiles. The effects of cleat geometry parameters, i.e., cleat spacings, aperture and heterogeneity, on permeability dynamics were further evaluated. The results demonstrated that i) cleat aperture exerts a significant influence on the magnitude of permeability variation but a subtle effect on the general evolution trend; ii) permeability variation trend is substantially affect by cleat spacing; larger cleat spacing tends to result in a U-shaped curve with decreasing rebound pressure; iii) permeability variation amplifies with stronger heterogeneity especially at higher pressures.

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Experimental Study on the Effect of Moisture on Adsorption and Desorption of Shale

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Adsorption is one of the important ways of shale gas storage. Study on adsorption and desorption characteristics of shale is an important basis for correctly evaluating the gas content and productivity of shale reservoirs. Shale is originally deposited in the water environment so that there is bound water in the micro/nano pores of shale reservoir. That is, adsorption and desorption of shale gas are actually presented under water-containing conditions. Backflow rate of fracturing fluid is low in the process of shale gas production by fracturing, and the retention of water base fracturing fluid can also cause a significant impact on the adsorption and desorption of shale. In order to study the effect of moisture on adsorption and desorption of shale gas, the adsorption and desorption experiments of shale samples with different water contents at different temperatures and pressures were carried out. We use the volumetric method of “one injection for more adsorption” to reduce experimental errors. The experimental results show that the adsorption and desorption of shale under water conditions satisfied Langmuir adsorption law, the maximum adsorption capacity was negatively linear with water content. With the increase of water content, the adsorption capacity of methane on shale decreases and the desorption hysteresis is more serious under the same pressure and temperature conditions, and meanwhile, with the increase of the experimental temperature, the adsorption amount of methane and the desorption hysteresis decreases under the same pressure and moisture conditions.

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Investigation of residual oil distribution and formation mechanisms at the extra-high water cut stage

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Oil fields in eastern China are normally entering into the extra-high water cut stage, and the poor effect of water flooding leads to the decrease in oil recovery. A large amount of residual oil remains trapped in reservoirs at this stage. To improve water flooding efficiency, it is necessary to understand the distribution and formation mechanisms of residual oil at the extra-high water cut stage. In this study, a pore-scale simulation model is developed to exploit the residual oil potential in a porous media. A direct numerical simulation method is employed to simulate the oil slug flow, the position of the interface between water and oil slug is determined using the phase field method. Finite element method is used to solve the model. The capacity and accuracy of the model is validated by a classical benchmark: a layered two-phase flow with a variable viscosity ratio. The results show that the residual oil in the porous media at the extra-high water cut stage can be classified as five types, namely, isolated oil droplet, residual oil in the pore throat, cluster residual oil, oil film and residual oil in the dead end. The formation mechanisms of residual oil are analyzed in terms of mechanics. Furthermore, the displacement curve is obtained based on the results of pore-scale simulation. It is also observed that the increase in injection velocity and the injection of surfactant can both improve the oil recovery in the porous media. Times of increasing injection velocity have an important pact on the field development. Under the same exploitation condition, the recovery of water-wet reservoir is higher.

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Microscale study of oil flow mechanism in tight reservoirs

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With the rapid decline in conventional reservoirs, unconventional reservoirs with huge reserve and extensive distribution, particularly like the tight oil and gas, are becoming more important to the global energy supply in the near future. However, the flow mechanism in tight reservoir is not very clear, especially for the tight oil. The oil flow may have different behaviors in microscale pore or throat. In this study, both experimental and numerical simulations are conducted. Firstly, simple models with different size channel are designed. During the simulation, the size of channel ranges from 5 microns to 500 microns. Different viscosity and injection rate are also considered. The relation between flow rate and pressure difference is studied in each model. At the same time, the numerical results are verified by the experimental results.

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Modelling and simulation of reactive dissolution during acidization of fractured carbonate rocks

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Acidizing is a commonly used stimulation treatment for carbonate reservoir by injecting acid into near-wellbore formation to remedy the damage and to create operational-optimal deep-penetrating and narrow high permeability channels, termed as wormholes, by mineral dissolution. Wormhole formation in un-fractured matrix has been widely studied by numerical modelling, but little work has been done for fractured cases which may cause wormholes to propagate quite differently. In this study, a continuum model with explicit fractures is developed, where the governing equations are discretized by the finite-volume method. This model produces the correct dissolution patterns on a 2-D un-fractured domain discretized by Delaunay triangulation. Then it is used to examine wormhole formation in cases with single, multiple, and complex fractures, including characteristics such as fracture orientation, aperture, connection, and distribution. It is found that neither the volume of acid required nor the dissolution structure is affected by fractures with small aperture. If the fracture aperture is large enough, the dissolution structure is dominated by the fracture distribution at intermediate injection rates but is independent with the fracture distribution at very low or very high injection rates. The presence of fractures and the increase of fracture aperture have no influence on the type of dissolution patterns. The volume of acid required to break through the core decreases with the increase of the fracture aperture, which is particularly noticeable when the dominate wormhole is created. For the fractured porous media of not well-connected fractures, the final dissolution structure of wormhole is determined by the fracture and matrix porosity distributions together. As for the well-connected fractures, the matrix heterogeneity has no contribution to the creation of the wormhole, and the dissolution front propagates along the fracture trace. Finally, for the field-scale application, it is found that the optimum injection rate is almost unchanged from un-fractured medium to fractured medium if the acid-mineral reaction system is same.

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Multiscale random walk simulations for computing effective electrical properties in heterogeneous rocks

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The electrical conductivity of heterogeneous rocks, such as carbonates or clay rich sandstones, is strongly dependent on the geometry and connectivity of its pore system. Complex depositional and diagenetic processes have a strong control on the pore structure, leading to systems with a very wide range of pore sizes covering many orders of magnitude in length scales, which cannot be captured by a single resolution micro-CT image. In the present work we present a multiscale imaging and modeling workflow to compute electrical properties of heterogeneous rocks. Dry and wet micro-CT images are used to spatially map the porosity and connectivity of macro- and micro-porous regions. High resolution BSE images are used to construct 3D models of different micro-porous regions. The electrical properties (cementation exponent) and statistical variability (heterogeneity) of the different micro-porous regions are determined from direct simulations on these high resolution 3D micro-porosity models. Furthermore, we distinguish between the effect of partially resolved grains (i.e. partial volume effects) and actual micro-porous regions. A new bounce back probability, based on the local porosity and cementation exponent, is calculated in each voxel of the porosity map in order to model the electrical conductivity of the non-resolved porosity regions. A direct random walk simulation is run on the 3D porosity map to determine the effective electrical conductivity and formation factor of the sample. This new multiscale methodology is validated using high-resolution detailed models and analytical solutions. Experimental and numerical results for carbonate and sandstone samples are compared and found to be in good agreement. Finally, the influence of the pore-scale heterogeneity on the electrical properties is characterized for each of the samples.

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Numerical Characterisation of Coal Fracture Systems and Prediction of Coal Petrophysics

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Coalbed methane reservoirs are important resources for natural gas that are gaining global interest due to their environmental benefit and abundance. Understanding the displacement of gas and water in coal seams, which is controlled by the microscale cleat system, is critical for explaining gas recovery processes. X-ray micro-computed tomography (micro-CT) is applied using a novel contrast agent method for visualising micrometer-sized fractures in coal. The technique allows for the visualisation of coal features not visible with conventional imaging methods. Then, cleat statistical information is extracted from micro-CT images to reconstruct coal cleat system numerically. This technique allows for preserving the key attributes of the cleat system while the generated fracture network is not limited in terms of size nor resolution. The cleat modelling method mimics the cleat formation process and preserves coal connectivity and cleat structure. Direct numerical simulations based on lattice Boltzmann methods are performed on the cleat network realisations to evaluate coal permeability. We show that directional permeabilities result in different system scaling effects because of the dependence on the underlying structure of the cleat network. The developed method facilitates the evaluation of the relationship between coal cleat structure and resulting flow properties, which are steps forward in the evaluation of coal petrophysical properties at the core scale. The reconstructed cleat system can be used for dynamic adaptive mesh simulations of multiphase flow of water and gas and upscaling of coal petrophysical properties including permeability and relative permeability. We discuss the advantages of the developed cleat reconstruction method for prediction of coal properties for large-scale reservoir simulation and evaluation of performance of coal seam gas reservoirs.

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Oil-Water Flow Simulation on Coupling Multiphysics Considering Steaming Potential

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The tight reservoirs have the characteristics of dense rock, low permeability and extremely small size of pore throats. Therefore, some interfacial forces neglected in conventional reservoirs can have a significant impact on fluid flow in these tight reservoirs. This thesis is mainly concerned with the study of the impact of the oil droplets on oil-water fluid flow in tight porous media of streaming potential resulting from the electrical double layer on the interface of grains and fluid. Models of coupled fluid flow in capillaries of constant radius considering steaming potential is established from the micro- and nanoscale to simulate oil-water fluid flow in tight porous media. The coupled Navier–Stokes equation, Poisson equation and Planck–Nernst equation are solved simultaneously to obtain the pressure distribution, the velocity profile, the distribution of electric potential and the concentration of ions in the model. The numerical results are then compared with that of the model which does not consider the electrokinetic coupling effects. According to the change of pressure and velocity of the oil droplets in the model, the force of electric coupling effect on the oil droplets on the wall of tight porous media is analyzed. The results suggest that streaming potential have some impact on the force state of oil droplets on the wall of tight porous media, which contribute to the study of oil droplets migration mechanism in tight reservoirs.

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Oil-Water Flow Simulation on Coupling Multiphysics Considering Steaming Potential

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Pore scale modelling of multiphase flow in mixed-wet porous media using a coupled Level Set with Volume of Fluid Method (CLSVOF)

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The wettability of fluid-rock system, which is established during reservoir formation and affected by mineralogy of the rock, the composition of the oil and water, the initial fluid distribution, and the temperature, have significant on multiphase flow (Zhou, et. al., 2013). Previously, several study have used network models to investigate the impact of wettability variation on flow at the pore scale (Blunt, et. al., 2013); however one main weakness of the network modelling is a representative pore-network is required prior to modelling, and thus it fails to capture the complexity of highly heterogeneous pore system and local wettability variation. Besides network modelling, direct pore scale modelling, such as Level set method (Jettestuen, et al, 2013) and volume of fluid method (Raeini et al., 2012), provide us an alternative approach to study wettability and its impact on flow. In this work, we proposed a CLSVOF method to simulate the multiphase flow in mixed-wet pore space that has been extracted directly from 3D rock images. In general, VoF is capable of predicting the evolution of free surfaces and this lies in its high volume preservative quality but still showing low accuracy in calculation of geometrical properties; while the LS method is highly accurate in predicting the interface evolution but still lacks sufficient precision in conserving the mass, and thus the newly proposed CLSVOF allow us to simulate multiphase flow with desirable accuracy. The open source fluid flow solver (OpenFOAM) is used as the mainframe for solving the PDE equations, and the variational level set method was introduced and coupled with the VoF to simulate the multiphase flow in mixed wet porous media. We first simulate the equilibrium fluid configuration in capillary tubes with both analytical and highly irregular cross section, and the simulated fluid configuration and entry pressure agree well with that from our semi-analytical approach (Zhou, et. al., 2013). This newly developed pore scale modelling approach was used to simulate the multiphase flow in 3D mixed-wet pore space. The simulation shows that the wettability distribution and pore geometry both acting on controlling the displacement processes.

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Pore Size Characterization and Adsorption Property Evaluations of Shales in China

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Abstract:Shale gas is one type of the unconventional natural gases which will play very important role in the future, especially for China. China has achieved great success in shale gas development in Sichuan Province after the USA shale gas revolution. Shale has different pore structure and different flow mechanisms. The mineral composition, TOC content were measured for the shale samples. The pore size and structure of shale samples were visualized by TEM and SEM methods. A new equipment was designed for the measurement of shale adsorption and desorption characteristics and the data were fitted by a new model. Experiments show that the shale samples are mainly composed of clastic minerals, clay minerals and authigenic brittle minerals; Organic carbon content (TOC) is relatively high in these shale samples; isolated nano scale pores can be observed in the SEM images. The adsorption capacity increases with the increase of equilibrium pressure and decreases with the increase of temperature and moisture; the adsorption capacity of different gases in turn is CO2 > CH4 > N2; the hysteretic characteristics of desorption is oberverd through the misalignment between adsorption isotherm and desorption isotherm. On the basis of the adsorption potential theory, a new model were constructed to fit the isothermal adsorption experimental data. Fitting results suggest that this new model has satisfied fitting effect and the fitting goodness are all above 0.99.The work is supported by the National Science & Technology major Project of China (No. 2016ZX05025-004-003), National Science Foundation of China（No.51234007） and Program for Changjiang Scholars and Innovative Research Team of China (No.IRT1294).

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Roughness Induced Oil Trapping in Microchannels

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Flow of a viscous fluid in a microconfinement is of significant importance in many of our daily life applications. E.g. enhance oil recovery (EOR) [1] includes processes such as waterflooding where crude oil is displaced by water in the porous matrix of the reservoir-rock. A lot of research effort has been spent in the past for studying oil water wettability of a solid phase and how it is influenced by the geometry of the porous medium [2]. Since the advent of microfluidics, various real life fluid displacement scenarios as well as the abovementioned oil-recovery related fluid flow/entrapment problems have been emulated in a microchannel [3]. While studying various pore-scale phenomena, the focus is usually on the complex processes involving capillary and viscous forces. However, the influence of the reservoir rock's roughness on the flow behavior is somewhat overlooked.

In this work, we investigate the effect of roughnesses upon the entrapment of oil (alkanes) by waterflooding in a microchannel. We use fluorescence microscopy in order to perform imbibition experiments and track the in-situ fluid displacement process in these channels. We find that the alkane viscosity determines whether the alkane phase will be retained in the microchannel. On the other hand, the quantity of the retained phase is determined by the roughness as well as the Capillary number (Ca) of the experiment.

Subsequently, we increase the complexity of the problem and perform the imbibition experiments in a 2D porous medium where the inherent roughness of a porous structure is considered. We observe that the trapped alkane in the porous medium follows the same trend as in the rough microchannels i.e., viscosity and roughness govern the trapped oil quantity. Usually, the trapped fluid volume in a confined pore/microchannel is described by a power law relating the Capillary number of the system . Here, we propose a general scaling law based on our experimental observations which integrate both the Capillary number as well as the characteristic roughness of the system to quantify the trapped fluid volume.

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Sensitivity Analysis of the effect of micro-fractures on petrophysical properties of tight reservoir

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Tight reservoir, as a typical unconventional reservoir, has attracted more and more attention all around the world. Compared with the conventional reservoirs, the pore-throat of the tight reservoirs is fine and the micro-fractures are developed and fluid flowing in the tight oil reservoir is very complicated. Therefore, the study of the influence of fractures on the rock topological structure as well as the flow characteristics between fractures and matirix is critical to the development of tight oil reservoirs. Due to the complexity of the fracture, digital rock analysis technology is employed to carry out this problem instead of the traditional experimental method. Firstly, the selected tight rock is scanned by CT, and then the real tight digital rock is obtained by filtering and binary segmentation. After analyzing the representative elementary volume (REV), it is found that the digital rock with the 4003 reservoir is enough. Finally, the fractures with different shapes are added to the digital core, and the pore network model extracted by the maximum ball method is adopted to conduct the simulation of flow. Results show that the ratio of fracture permeability and matrix permeability along the fracture conduction direction has an exponential relationship with the fracture aperture, shows a linear relationship with the length of the crack as well as the cosine of the fracture inclination angle, and has nothing to do with the crack trend. The ratio along the disconnected direction doesn't relate with the fracture aperture, fracture length and fracture inclination angle, but appears symmetrical change on the both side of the crack trend. The residual oil saturation has an exponential relationship with the crack aperture, shows a linear relationship with the the crack length, and presents no connection with the crack trend and dip. As the existence of fractures, the distribution of pore radius and roar radius is changed from a typical single peak to bimodal mode.

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Shear-thinning or shear-thickening for better EOR? -- A direct pore-scale study

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Non-Newtonian fluids are widely applied in Enhanced Oil Recovery (EOR) techniques, and the shear-thinning or shear-thickening behavior is one of the most common features of them. However, there seems to have some debates on which category is better [1-3]. Direct pore-scale methods like OpenFOAM and lattice Boltzmann method (LBM) have offered an alternative powerful way for revealing flow physics in porous media. Nevertheless, few relevant studies on this specific issue have been found, except some indirect investigations on single-phase non-Newtonian fluid flow in porous media. In this paper, we aim at discovering the roles of these rheological properties in non-Newtonian fluid displacement strictly from the pore scale. A recently developed lattice Boltzmann model (LBM) for multiphase viscoplastic fluid flow [4] is used. This model is able to capture the momentum evolution and yielded regions well in two-phase non-Newtonian flow. The localized treatment of shear rate in this LBM model can improve the efficiency and accuracy over other direct simulators, thus make it suitable as well for direct flow simulations in porous media. Displacements in both homogeneous and heterogeneous porous media are considered. For homogeneous cases, we found the performance of shear-thinning and shear-thickening fluids are almost the same when compared in favorable displacement regime; while the performance of shear-thinning fluid is poorer than shear-thickening fluid in unfavorable displacement regime. For heterogeneous cases, we demonstrate that the shear-thinning property does not contribute too much on the diversion effect, which corrects some of the previous understandings. Our results still indicate the significance of low mobility ratio for diversion and EOR, which can stabilize the displacing front although may increase the viscous resistance. Therefore, we further discuss how to determine an optimal viscosity ratio to balance the oil recovery and energy cost with economic consideration in the end.

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Simulation of the gas transport in reconstructed random micro-porous media by the lattice Boltzmann method

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In recent years, the rapid development of the Microelectromechanical systems (MEMinisymposium), the fuel cell technology, and the unconventional gas reservoirs has raised the necessity for a deeper understanding of gas flow behavior in micro-porous media. In these systems, the characteristic pore size is in the same order of magnitude as the mean free path (λ) of the gas molecules, and according to the Knudsen numbers (Kn), the gas flow is found to be dynamically similar to rarefied gas flows. Although the computational fluid dynamic (CFD) approaches have been successfully applied to simulate hydrodynamic flows in porous media, and some extensions have been made to simulate rarefied gas flow in simple geometries, their applications to micro-gaseous flow in complex disordered porous media remains an open problem. In this paper, different porous structures are reconstructed in two dimensions by employing the quartet structure generation set approach (QSGeneral Session) [1] (See Figure 1). The lattice Boltzmann method is adopted to simulate gas transport in micro-porous media, and the multiple-relaxation-time collision operator is applied. To implement the model correctly, the regularization procedure [2] is induced to overcome the nonphysical momentum oscillations around the solid obstacles, and all the porous inter-facial nodes are recognized and classified into different types. In addition, a modified power law (PL) based wall function approach is implemented to calculate the local mean free path of gas molecules in confined pore space. A comparative flow simulation study indicates a general agreement of predicted velocity profiles between molecular dynamic (MD) and that proposed LB model. Next, a number of simulation studies of gas transport through series reconstructed structures are carried out, and the results reflect that the rarefication greatly affects the gas transport in porous media (See Figure 2) and the apparent permeability decreases with the pore pressure. In addition, both the pore configuration and tortuosity control the velocity profile and the estimated apparent permeability. It has been observed that gas transport behavior in complex structures such as the one presented in Figure 1(a) deviates significantly from that in uniform channels. The present study provides a comprehensive theoretical and practical guidance for the designing and optimizing of numerical simulators for unconventional gas reservoir.

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Studies of corner flow using lattice Boltzmann method

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Capillary processes in porous media can show a meniscus moving across pores, but also in the roughness or corners of the pore space. In simple geometrical systems, capillary uptake is often studied with fluids wetting a cylindrical tube showing a pore meniscus. However, flow can also spontaneously occur at the intersection of two planes forming an angle smaller than the wetting contact angle of the fluid on the solid. In polygonal capillary tubes, the number of sides defines a critical contact angle,ni.e. theta-critical, which controls two configurations of fluid transport: the formation of a pore meniscus at theta larger than theta-critical or the occurrence of corner arc menisci at theta smaller theta-critical (see Figure 1a). The latter phenomenon has received different names in the literature where we retain here the term corner flow.

We study the water behavior in individual pores or systems of pores using lattice Boltzmann modeling (LBM) (Chen et al. 2014) to capture the movement of the liquid/gas interface and to particularly analyze a still challenging unsaturated-state phenomenon, namely corner flow (Figure 1b and Son et al. 2016).

In new studies, similar corner flow processes, regardless of the specific corner path, are found in the following configurations: straight path, straight path with U-bent and staircase path. This shows that corner flow is resilient and independent of path configuration.

Figure 1. a) Schematic representation of the two liquid configurations in a square tube: (a) pore meniscus when the contact angle is larger than the critical contact angle, theta larger than theta-critical; and (b) co-occurrence of pore and corner arc menisci when the contact angle is smaller than the critical contact angle, theta smaller than theta-critical, b) Liquid configuration versus time at different iteration count for theta equal 22 degrees in a square tube (from Son et al. 2016)

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The experimental study on the flooding regularities of various CO2 flooding modes implemented on ultra-low permeability cores

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Due to the fine pore sizes, it's very difficult to exploit low-permeability reservoirs, especially the ultra-low- permeability reservoirs. And due to the difficulty of water injection operation, the conventional water flooding recovery is too far to be satisfactory. However, because of the special properties of CO2, CO2 can dissolve readily in crude oil and the oil mobility can be highly improved, which makes CO2 flooding an effective way to the development of the ultra-low-permeability reservoirs. In this paper, the regularities of various CO2 displacement methods are studied via experiments implemented on the ultra-low-permeability cores from Chang 8 Formation of Honghe Oilfield in Southern Ordos. The experiments were performed under the formation conditions of Chang 8 reservoir. The results show that: CO2 miscible displacement method has the minimum displacement differential pressure and maximum oil recovery; CO2-alternating-Water miscible flooding method has lower oil recovery, higher drive pressure and relatively lower gas-oil ratio; Water flooding has the minimum oil recovery and the maximum driving pressure. A large amount of oil still can be produced under a high gas-oil ratio condition through CO2 displacement method. This fact proves that the increase of gas-oil ratio is caused by the production of dissolved CO2 in oil rather than the free gas breakthrough. At the initial stage of CO2 injection, CO2 doesn't improve the oil recovery immediately. But as the injection continues, the oil recovery can be improved rapidly. This phenomenon suggests that when CO2 displacement is performed at high water cut period, the water cut doesn't decrease immediately and will remain high for a period of time, then a rapid decline of water cut and increase of oil production can be observed.

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Three dimensional effects in flow through thin porous media

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Stationary incompressible fluid flow in a thin periodic porous medium is considered. The medium under consideration is a bounded perforated 3D-domain confined between two parallel plates. The distance between the plates is δ, and the perforation consists of ε- periodically distributed solid cylinders, which connect the plates in the perpendicular direction. Both parameters ε, δ are assumed to be small in comparison with the planar dimensions of the plates. By such an approach homogenization analysis for low Reynolds number flows show that when $\delta << \varepsilon$ and $\varepsilon << \delta$ the flow can be treated with a 2-dimensional approach while when δ and ε are of similar size the problem is 3-dimensional. In the current study the theory is challenged by tomographic-Particle Image Velocity full 3-dimensional measurements for a wide range of Reynolds numbers and ways to extend the theory to higher Reynolds numbers are outlined.

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Upscaling of gas transport in multiscale shale samples based on homogenization theory

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Traditional gas transport model could not describe the complex gas transport in shale sample with multiscale pore spaces involves organic matrix, inorganic matrix and micro-fracture network. In this paper, a upscaled macro-scale model by two steps upscaling processes is established to describe the gas transport in multiscale shale samples composed of matrix and fracture network. In the first step, a upscaled matrix model is adopted in the meso-scale region to investigate the gas flow in matrix with considering the kerogen distribution. In order to investigate the interaction between the matrix and the fractures, the fracture system is coupled with the matrix model, and then an upscaled macro-scale model is established by using homogenization theory. Several schemes are conducted with different fracture network distribution in the meso-scale region while has the same parameters in the macro-scale model. The numerical results show the solved pressure and production with upscaling process are different in the macro-scale models while the macro-scale equations without homogenization process have the same pressure and production. The work indicates that the upscaling process of gas transport in shale samples with multiscale pore spaces is necessary to obtain more accurate numerical simulation results.

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A TPM-based Investigation of Fracking Processes in Saturated Porous Media

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Hydraulic fracturing in porous media, such as soil and rock, came into play in the late 1940s and found its application in the oil and gas industry, the exploitation of deep groundwater sources and deep geothermal energy plants. Fracking in non-saturated and saturated porous media is an important area of research, since these methods are widely used in practice. In contrast to the application of fracking techniques, the theoretical and computational description of this method, especially in saturated soil and rock, is still in its infancy.

To overcome this situation, the present contribution aims at describing the basic fracking process in saturated porous materials. The derivation is based on the well-founded Theory of Porous Media (TPM) [1] and includes a permeable rock-like material saturated with water. Evolving cracks as a result of fracking [2,3] are included in the description by enhancing the TPM by the phase-field approach to fracture [4], where the phase field itself is used for the detection and evolution of single cracks and crack fields, which are mainly driven by the pressure of the fracking fluid.

By use of the solver PANDAS, which has been created for the solution of strongly coupled problems in extended continuum mechanics, numerical examples with 2-dimensional and 3-dimensional geometries exhibit the possibilities of the overall procedure.

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Effect of anisotropy and heterogeneity on hydraulic fractures

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Hydraulic fracturing has been an important enabler for the profitable extraction of oil and gas from the unconventional reservoirs, namely shales. It is important to model the hydraulic fracture process for decreasing the environmental footprint as well as enhancing productivity by creating less fractures in a much more efficient way. Several models have been proposed for this purpose, but most of them do not take into consideration the anisotropy and heterogeneity present in shales. In this model, we make use of a two dimensional extended finite element model (XFEM) with an enhanced local pressure (ELP) proposed by Remij et. al. [1] to include anisotropy and heterogeneity. In shales, clay platelets are oriented along a particular direction making the properties vary in different directions. The anisotropy in properties such as Young's Modulus, Ultimate tensile strength and permeability along with crack initial orientation and the anisotropy in loading determine the magnitude and orientation of the hydraulic fracture. The two major factors influencing are the Young's modulus, which promotes fracture growth perpendicular to the grain direction, and the ultimate tensile strength, which promotes fracture growth parallel to the grain direction. In figure 1, we see a vertical hydraulic fracture with equal loading in both directions and 50% anisotropy in the material properties for various grain orientation angles. We can observe that the crack always gets oriented along the grain direction. In figure 2, we see three cracks with different initial orientations (0 ,60 ,90) with equal loading and 50% material anisotropy at a grain orientation angle of 60. Irrespective of the initial orientation direction, all the three cracks align along the grain orientation angle. The heterogeneity can be classified into two types: a) Point-wise heterogeneity, where properties vary from point to point. These maybe due to the natural variation in rock properties which is more gradual or also due to various impurities or inclusions within the rock. b) Layer-wise heterogeneity, where properties vary from one layer to the other. This is due to the gradual formation of rocks over long periods of time, which causes the rock properties to vary from one layer to the other generally in the vertical direction. In figure 3, two cases of effect of inclusions on the fracture propagation is illustrated. When the inclusions or concretions are harder than the original rock the crack gets deflected away from them, in case of softer inclusions the crack gets attracted towards them.

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Experimental Study of Thermal fracturing of liquid-saturated rock under HPHT

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During oil- and geothermal-field development, CO2 geological sequestration, and nuclear waste underground storage, the reservoir will undergo dramatic temperature changes. Such changes result in thermal expansion or contraction within rocks and induce abundant micro-fractures. In return, this thermal fracturing process will affect the flow of fluid and temperature distribution in porous media. Therefore, it is critical to understand the mechanisms of thermal fracturing for different rocks. In this paper, we present the experimental study results of thermal fracturing in a controlled laboratory environment. It provides an insight to physical changes that may be expected at the field practice, and assists in securing reservoir integrity and optimizing reservoir management. When designing the experiment apparatus, we considered the actual displacement process in the high pressure and high temperature (HPHT) environment. The apparatus was developed to heat rock cores from one of their ends rather than heating the sample evenly as a whole piece. The heating rate can be adjusted and the highest temperature is 600℃ at up to 40MPa confining pressure. Also, cold liquid was injected to simulate the rapid quenching process. Four rocks from oil and gas formation were heated and quenched to simulate thermal fracturing process and test our methodology. Microstructure, porosity, permeability, mineral components, and acoustic emission are used to characterize the physical changes of rock which experienced thermal fracturing. Results indicate that the porosity and permeability of rock increased, and the fracture network within rocks developed and matured. Compared to the dry and whole heating, the presented saturated and end heating will result in more damage in rocks.

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Finite element modeling of hydraulic fracturing using the PFM approach

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Fracturing of porous materials is a very important subject in various branches of engineering. To give some examples, consider in the energy sector the enhanced geothermal systems (EGeneral Session), that are applied to generate geothermal electricity. In this, high-pressure fluids are injected into deep rock layers with low permeability in order to enhance the rock's permeability and, with this, improving the system's efficiency. Additionally, hydraulic fracture is used in petroleum engineering to extract shale gas.

In this research work, the numerical modeling of fracture in saturated heterogeneous materials is carried out using an extended form of the continuum Theory of Porous Media (TPM), which accounts for the crack nucleation and propagation, deformation of the solid matrix and change in the flow of the interstitial fluids. The extension towards fracture modeling succeeds using the energy-based phase-field modeling (PFM) approach, see e.g. [1]. Starting with the mathematical modeling and material description of fluid-saturated porous materials using the TPM, the proposed treatment assumes steady-state behavior (quasi-static) and neglects the chemical effects as well as any mass exchange between the solid and fluid constituents. This leads to a strongly coupled system of differential algebraic balance equations (DAE), which demands special numerical schemes for a stable solution. On the other hand, the PFM is a diffusive crack-interface approach that allows simulation of microstructural evolution such as crack propagation on a macroscopic scale. In this, once the critical energy release rate is reached, a crack, associated with local degradation of stiffness, takes place [2].

To reveal the ability of the proposed modeling strategy in capturing the basic features of hydraulic fracture, numerical examples using the finite element method will be presented.

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Poro-mechanics of Confined Electrolytes in The Context of Freeze-thaw Damages

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Cementitious porous media are long known to be vunerable to freeze-thaw cycles. Damages from these cycles are associated with the high degree of saturation, porosity and connectivity of the pore network, amount of air voids in the meso-scopic structure and usage of de-icing salts. The depression of freezing point (e.g. the Gibbs-Thomson equation) in nano-pores suggests that under normal freezing temperatures (-10 C) only in large pores (>20 nms) the liquid water turns into solid ice while in smaller nano-pores water will remain liquid state. Thermodynamically there will always be a very thin (~ 1 nm) lubricating layer of liquid between the ice core and the CSH (the solid component of cement) matrix. Given a constant temperature, ice can stand a quite large melting pressure (~ 100 MPa) before it melts. Our molecular simulations indicate that the confined counter-ions and electrolytes in the lubricating layer of liquid can give rise to a large disjoining force. Below the ice melting pressure this force is carried by the solids (ice and CSH) in the system and potentially generates micro-crackings. In our simulations we compare the forces generated by point charge ions with both the DLVO theory and the Wigner Crystal (WC) expansion. We go beyond these theories by including finite ion size as well as fluctuation and correlations of ions. Later we include water molecules and electrolytes explicitly and discuss possible surface adsorption effect induced by pollution of charged large chemical groups. Finally we will demonstrate the percolation of ice growth and micro-crackings with a meso-scopic model of cement porous structure.

Figure 1: The Virial pressure measured from the ions (and electrolytes) in the confined asymmetric configurations. X-axis is the distance between ice surface and CSH surface. Black curves are the theoretical calculations of DLVO and WC approximations. Figure 2: A snapshot from the very confined and asymmetric ice-electrolyte-CSH simulated structure. Meaning of particle colors: green—ions; yellow—CSH surface charge; dark green—ice surface; red—symmetry plane. The system is periodic in the x-z plane. The systems will evolve in 1 million time-steps and then physical quantities measured and averaged in the next 1 million steps. Figure 3: A snapshot for the percolation of ice and micro-cracking growth. Dark particles represent CSH and blue particles represent ice.

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Ion transport in heterogeneous charged nanoporous media and non-linear electrokinetic effects

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The heterogeneous charged nanoporous mediums could be found in different aspects in nature from geology to biology. It is well known that the surface electrical charge is dependent to the local environmental properties like pH, ionic strength, temperature and either the pore structure. While the pore scale study would be focused on scales comparable with the electrical double layer thickness, consequently, the strong non-linear electrokinetic effects would be emerge as a key parameter. In most of the previous studies, either in large scale or pore scale, a homogeneous charge has been applied on solid-liquid interfaces. However, the effects of heterogeneous charge on electrokinetic transport in porous media has been seldom studied because it poses bottlenecks in, on one hand, proposing appropriate models to connect surface charge with local physical properties, and on the other hand, solving governing equations for transport in complex geometry like porous media with efficient numerical methods. The aim of this study is to, first, propose a modified electrical triple layer (METL) model which is suitable to predict the zeta potential locally for low to high ionic strength in the pH range of 3-9. Second, the heterogeneity of the electrical charge in porous medium would be defined by modeling the electrokinetic transport of ions while it could be strengthen by imposing pH or concentration gradient. Third, the heterogeneous charged pores may impose strong local non-linear electrokinetic phenomenon which would be influenced the electrokinetic transport in porous media. In this study, the coupled Navier–Stokes, Poisson and Nernst–Planck equations are iteratively solved by multiple lattice Boltzmann methods (LBM) to obtain the velocity, internal electric potential and ion distribution, respectively. The METL model would be solved for each solid-liquid surface node in order to obtain the local electrical charge as boundary condition for Poisson equation. The 3D porous structures are reproduced by using the random generation-growth method which is suitable for generation of random microstructure porous media.

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Effect of wind characteristics on gas dispersion in porous media

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Greenhouse gases have the key role in global warming. Soil is a source of greenhouse gases such as methane (CH4). Radon (Rn) which is a radioactive gas can emit form soil into the buildings and causes health concerns. Different soil properties can affect gas emissions inside/from soil including temperature, humidity, air pressure and vegetation (Oertel et al., 2016). It's shown in many cases that pressure fluctuations caused by wind play an important role in transport of gas in soil and other porous media. An example is: landfill gas emissions (Poulsen et al., 2001).

We applied a novel experimental equipment for measuring controlled wind turbulence on gas transport in porous media. This set-up was utilized to evaluate the effect of wind turbulence on gas transport in relation to the depth of porous medium. Experiments were carried out with binary diffusion of CO2 and air as tracer gases with average vertical wind speeds of 0.02 to 1.06 m s-1. 13 different wind conditions with different speed and fluctuations were applied. Five oxygen sensors were places inside sample at different depths to measure air transportation within porous media and total of 39 experiments were carried out.

Gas transport in porous media is described by advection-dispersion equation. Gas transport is quantified as a dispersion coefficient. Oxygen breakthrough curves as a function of distance to the surface of the porous medium exposed to wind were derived numerically with an explicit forward time, central space finite-difference based model to assess gas transport.

We showed that wind turbulence-induced dispersion of gas is an important transport mechanism that can increase gas transport with average of 45 times more than molecular diffusion under no-wind condition. Power spectrum density is calculated for all the 12 wind conditions to determine strength vibration of all the wind speeds.

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Efficient and accurate numerical model for Density Driven Flow in unsaturated porous media

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Modeling Density Driven Flow (DDF) in unsaturated porous media requires the coupling between the Richards and the mass transport equations. Due to its nonlinearity and intrinsic complexity, the numerical solution of such a coupled system of equations has not been greatly investigated in the literature. Most of the exiting numerical solutions are based on standard numerical methods for space discretization (Finite element or Finite volume methods) with the first backward Euler scheme for time integration [1, 2]. Coupling between flow and transport equations is usually performed via a sequential approach. However, standard methods have a limited capacity to represent reality and can lead to inaccurate results especially when real field configurations (heterogeneity, anisotropy, large space and time scales) are used in the simulations. In the case of saturated flow condition these numerical errors are unproblematic even if they affect the accuracy of the numerical solution. For unsaturated flow some numerical errors (i.e. unphysical oscillations) can lead to the divergence of the nonlinear resolution procedure. Furthermore, accurate integration with first order schemes imposes strict and severe constraint on the time step size and sequential approach has a slow rate of convergence [3]. The objective of this work is to develop a new efficient and accurate numerical model for DDF in unsaturated porous media that allows simulating practical applications under realistic conditions. The main idea is to couple advanced methods for spatial discretization (Mixed Hybrid Finite Element method, Discontinuous Galerkin Finite Element method and Multi Point Flux Approximation method) with higher order time integration techniques via the Method of Lines (MOL) [4]. This method proceeds by converting the partial differential equations into a system of ordinary differential equations by discretizing only the spatial derivatives and maintaining the temporal derivatives in the continuous form. The resulting ODE system can then be solved using higher order adaptive integrators. For the MOL implementation, the flow and transport equations should be solved simultaneously into a single step. This aspect is essential for MOL implementation and avoids slow convergence encountered with the sequential approach. The ability and efficiency of the new developed model to treat real field conditions are highlighted through the simulation of seawater intrusion in a coastal aquifer in Lebanon at the regional scale.

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Experimental and numerical investigation of the shapes of spontaneously emerging dissolution structures in porous rock

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Dissolution fingers (or wormholes) are formed in porous medium due to positive feedback between transport of reactant and chemical reactions [1-3]. Local changes in pore geometry due to the dissolution result in a variation of permeability, focusing the flow and leading to further increase in chemical erosion.

We study dissolution in a simple microfluidic setup, with a gypsum block inserted in between two parallel polycarbonate plates forming a Hele-Shaw cell [4]. By changing the flow rate and the distance between the plates we can scan a relatively wide range of Péclet and Damkohler numbers, characterizing the relative magnitude of advection, diffusion and reaction in the system. The wormholes are found to have highly regular forms of two different kinds: either needle-like (for large flows) or parabolic (for small flows). Both advance into the system with a constant velocity. We show that the velocities of the parabolic forms are equal to these of a planar dissolution front. The linear fingers, on the other hand, advance with the speeds inversely proportional to their widths. Next, combining numerical simulations with analytical modeling, we find the shapes of stationary, invariantly propagating wormholes for different widths of the system, flow rates and reaction rates.

Finally, we consider the problem of a dissolution of finite-sized objects immersed in a flow. Also in this case the experiments show a number of unexpected regularities. In particular, the upstream (trailing) edge of the dissolving object is shown to advance with a constant velocity. These results are also confirmed in numerical simulations.

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Extended Macroscopic Description of non-Wetting Liquid Intrusion into a Ball of Porous Material

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The problem of macroscopic description of quasi static intrusion of non-wetting liquid (mercury) into a ball of porous material is considered. A new macroscopic description is proposed for quasi static process of non-wetting liquid intrusion into a ball of porous material. The analysed problem is an extension of the description presented in the paper [1]. Considerations are based on the continuum model of the capillary transport of liquid and gas in unsaturated porous materials, proposed by one of authors of the present paper, [2]. The key assumptions of this model are: division of liquid in the pore space into two macroscopic constituents called mobile liquid and capillary liquid; description of menisci motion by an additional macroscopic velocity field; parametrization of saturation changes by a macroscopic pressure-like quantity that for quasi static and stationary processes is equal to the capillary pressure. The capillary liquid forms a film on the contact surface with the skeleton. This liquid is immobile and contains the whole interfacial (capillary) energy of liquid in the pore space. The remaining part of the liquid surrounded by the layer of capillary liquid and menisci forms the mobile liquid. Both liquids exchange mass, linear momentum and energy in the vicinity of menisci surfaces and this occurs only during menisci motion in the pore space. For all constituents of the porous medium, balance equations of mass, linear momentum and energy are formulated and constitutive relations for mechanical processes are derived. Based on equations of this theory, equations for the quasi static process of non-wetting (mercury) liquid intrusion into porous materials were derived. It is assumed in the present paper that pressure of mercury surrounding the ball is equal to zero at the beginning of the intrusion process and the ball pore space is empty (vacuum). The increase of pressure in mercury causes penetration of mercury into pores of the ball and its spatial distribution that evolve during the process of mercury intrusion. The quasi static process of mobile liquid intrusion into a ball porous material is the special case of the model presented in the paper [2]. This process is described by strongly nonlinear evolution equation for saturation distribution with the mobile liquid. The boundary condition on the ball surface defining its saturation, depends on the mercury pressure and the pore diameter distribution. Equation describing this process is solved analytically for special forms of transport coefficients using the method of characteristics. This enables to derive expression for the so called capillary pressure curve defining dependence of ball saturation on the mercury pressure, and to analyze its dependence on diameter of the ball and parameters characterizing liquid transport in the pore space and pore size distribution.

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Fast Adaptive Implicit Methods for Multicomponent Compressible Flow in Heterogeneous and Fractured Porous Media

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Flow and transport in fractured reservoirs is one of the most challenging problems to model in hydrocarbon reservoir engineering and hydrogeology because of the orders of magnitude range in rock properties, flow rates, and spatial dimensions. Porosity and permeability heterogeneity, e.g. layering, pose similar challenges. Numerical approximations to the mass conservation equations that are explicit in time are conditionally stable and suffer from stringent constraints on time-step sizes. Implicit methods allow for large time-steps but also introduce high numerical dispersion. We compare explicit and new fully-implicit and adaptive-implicit methods for a discrete fracture model of multicomponent compressible flow. Both lowest-order finite volume (FV) and second-order discontinuous Galerkin (DG) methods are developed and coupled to a Mixed Hybrid Finite Element method for the velocity and pressure fields. The adaptive implicit methods (AIM) are adaptive in both space and time. For fractured reservoirs, fractures and near-well regions are typically updated implicitly, while most of the grid blocks in the matrix can be updated explicitly. This results in a scheme that is more efficient in terms of CPU time and storage requirements than a fully implicit approximation, while keeping numerical dispersion low. We also demonstrate the strength of AIM in modeling flow instabilities in relatively uniform porous media for which our AIM approach automatically tracks the front of viscous and gravitational fingers. A range of numerical examples is presented that demonstrate gains in CPU efficiency by 1 – 3 orders of magnitude by using DG-AIM. This allows one to accurately model large-scale 3D flow and transport problems in heterogeneous and fractured reservoirs that would be prohibitively expensive with methods that have high numerical dispersion and thus would require mesh refinement for comparable accuracy.

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Finite-element model to simulate buoyancy driven mixing in porous media

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We present a time- and cost-effective tool for researchers to design porous medium density fingering experiments with analogue fluids. Dissolution trapping of CO_2 in saline aquifers has been identified as a potential mechanism to prevent CO_2 from escaping to the atmosphere. To better understand the characteristics of this CO_2 trapping mechanism and to estimate the dissolution flux of CO_2 into brine, researchers perform lab experiments using analogue fluids in a Hele-Shaw cell (e.g. Neufeld et al. 2010 [1]) or cylindrical cell (e.g. Wang et al. 2016 [2]) filled with beads to simulate a porous medium.

Experimental work with analogue fluids can provide invaluable insights. However, scientists usually need to perform many experiments before they could find the parameters exhibiting the desired effects and validate the reproducibly of the results. Making the process time consuming and expensive. Furthermore, there is not yet a consensus amongst the scientific community what the practical measure is to estimate the dissolution flux. The one uses the receding interface velocity e.g. [1], while another the finger-extension velocity e.g. [2]. This leads to inconsistencies. Finally, experimental results are often compared to idealised 2D simulations, where the simulation system size is usually different from the experiment while keeping the Rayleigh number the same, however the fluid dynamic effects arising from the additional spatial dimension and walls are completely ignored.

We have developed a finite element model to simulate the relevant mixing dynamics of density fingering in porous media. In this model, we estimate the permeability of the bead pack using the Kozeny-Carman equation and the flow field is coupled to the transport of species. We performed two- and three-dimensional simulations, as shown in figure 1, and computed the dissolution flux using the receding interface velocity and finger-extension velocity, we denote the corresponding flux as, respectively, J_1 and J_2. We scale these with the diffusive flux: J_{dif} = (\phi D)dC_{max}/H_B, where (\phi D) is the effective diffusion coefficient of MEG, dC_{max} the maximum concentration difference i.e. dC_{max} = [\rho_f*X_{MEG}]_{max} and H_B the height of the bottom domain, to calculate the Sherwood number: Sh_i = J_i/J_{dif}.

We found that Sh_1 scales linearly with the Rayleigh number (Ra) at the constant flux regime: Sh_1 = 0.091*Ra^{0.91} for 2D and all 3D simulations. However, Sh_2 (as a function of Ra) varies with W/L as a result of walls and effects arising from the additional spatial dimension. Therefore, we suggest to use J_1 as the measure for dissolution flux in analogue fluids experiments. Finally, the model is used to predict the mixing dynamics of a MEG-Brine system in a bowl geometry as shown in figure 2. The bowl is filled with glass beads of a diameter of d_p = 0.5mm. The top domain is filled with MEG + KI and bottom domain is saturated with brine (water + NaCl). The experimental result is obtained using our in-house Medical-

CT scanner with a voxel resolution of ~1mm. Good agreement of the dissolution flux of MEG into brine, J_1, is found between the experiment and simulation.

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Improved Modeling of Gravity Aided Spontaneous Imbibition Using Momentum-Equation Based Relative Permeabilities

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It is well known that relative permeabilities (RPs) can vary depending on the flow configuration and are lower during counter-current flow as compared to co-current flow. Using a novel momentum-equation approach to generate effective RPs this dependence is well captured whereby the fluids transfer momentum due to fluid-rock interaction and fluid-fluid interaction. During co-current flow the faster moving fluid accelerates the slow fluid, but is itself decelerated, while for counter-current flow they are both decelerated. The decelerated fluid obtains a reduced RP, and the accelerated fluid obtains an increased RP resulting from this interaction effect. We present an application of this model where interaction-effects are significant and required to correctly predict different stages of oil recovery. The model is parametrized to fit experimental data. We consider recovery of oil from a mixed-wet matrix block surrounded by water due to a combination of gravity drainage (GD) and spontaneous imbibition (SI). The geometry is 1D vertical. At early times the flow is mainly counter-current due to SI, while for late times the process is co-current dominated. This is reflected in increasing RP curves with time. The full range of recovery regimes can only be captured using the momentum-equation approach. Using fixed RP curves obtained from a co-current configuration, as measured in the lab, can result in significant errors: in particular, the recovery rate will be overestimated throughout the recovery period. Further, large blocks are more dominated by GD and co-current flow with high RP curves. Small blocks are more dominated by SI and counter-current flow with reduced RP curves. Using one set of parameters the momentum-equation model is able to model the behavior of blocks of different sizes.

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In-depth analysis of hydrodynamics and conjugate heat transfer in solid sponges by means of a pore-scale CFD model

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Solid sponges are open-cell, highly porous ceramic or metal foams with a large specific surface area. These advantageous intrinsic properties promise very high heat and mass transfer rates at comparatively low pressure drops. A more specific advantage of sponge structures with regard to heat transfer is the continuity of their solid matrix. This allows for continuous heat conduction throughout the whole solid structure and, therefore, for a much more efficient overall heat transfer mechanism between the porous medium and its interface to the surrounding. Provided that these bi-continuous porous media conduct heat well, they offer superior heat transfer characteristics as compared to conventional packings which are subjected to multiple additional contact heat transfer resistances. This is why sponges are already used or considered for heat-intensive applications today, such as porous burners and volumetric solar receivers. This work presents a pore-scale CFD modelling approach to investigate single-phase hydrodynamics and heat transfer in sponges and similar irregular, bi-continuous porous media. The simulation geometry is derived from micro computed tomography (µCT) scans of the original sponge structure. To obtain reliable numerical results at a reasonable computational cost, adequately sized and shaped representative elementary volumes (REVs) of the structure need to be chosen and reconstructed. In the present case, cylindrical REVs of ceramic SiSiC sponge samples have been chosen for the numerical study (see Fig. 1a). Depending on the flow velocities investigated and, thus, on the flow regimes expected inside the porous medium, both steady-state and transient flow solvers have been used [1]. The latter includes both laminar and Large Eddy Simulation (LES) turbulence modelling approaches to account for the respective flow characteristics. Heat transfer calculations have been based on two different modelling approaches. The first of them considers the convective heat transfer of the fluid only and, thereby, assumes that thermal boundary conditions are provided, whereas the second approach includes heat conduction of the solid matrix in a more elaborate conjugate heat transfer model. CFD results have been compared to corresponding experimental results for pressure drop and volumetric heat transfer coefficient and showed good agreement [2]. Given the reliability of the CFD model developed, numerical results have been used to provide further in-depth insights into the transport processes prevailing inside the porous medium (see Fig. 1b). For example, form drag and skin friction drag contributions to the overall pressure drop have been analyzed as well as the influence of boundary conditions and flow regimes on momentum and heat transfer. These findings help to gain an improved understanding of the underlying transport phenomena and might be used to identify particularly favorable geometrical features of the porous structure and to optimize them for specific heat exchanger applications.

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Influence of chemical reactions on the convective dissolution of carbon dioxide in porous media

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Dissolution-driven convection in partially miscible systems has regained much interest in the context of CO2 sequestration [1,2]. A buoyantly unstable density stratification can build upon dissolution of CO2 into brine, thereby driving convection. Dissolution and convection are known to improve the safety of the sequestration process by reducing the risks of leaks of CO2 to the atmosphere. The question remains, however, as to how the efficiency of such process depends on the chemical properties of the storage site.

Chemical reactions can indeed affect convective instabilities as they modify concentrations and thereby the density profiles building up in the fluid [3]. We here show that a chemical reaction of CO2 with a dissolved chemical species can either enhance or decrease the amplitude of convection compared to the non reactive case. We use direct numerical simulations of Darcy's equations coupled to reaction-diffusion-convection equations to classify the various possible cases as a function of the contributions to density and diffusion coefficients of the chemical species involved. We discuss the impact of chemistry on the interfacial flux of CO2 and the time scales needed for its dissolution in aqueous solutions.

We illustrate our numerical findings by experimental results showing that reactions accelerate the development of buoyancy-driven fingering during the convective dissolution of CO2 into aqueous reactive solutions of alkali hydroxides [4].

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NEWTONIAN FLUID FLOW PAST A PERMEABLE STRETCHING/SHRINKING SHEET IN A POROUS MEDIUM

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In this talk, Newtonian fluid flow past a permeable stretching/shrinking sheet embedded in a porous medium using a proposed Brinkman model. The governing system of nonlinear partial differential equations describing the problem is converted to a system of non-linear ordinary differential equations by using the similarity transformations. Analytical solution is obtained for velocity. The effects of the Brinkman number or viscosity ratio, slip parameter, Darcy number, suction/injection parameter and the mass suction parameter on the velocity distribution are presented graphically and discussed. The results have possible technological applications in extrusion process and such other allied areas and in the fluid based systems involving stretchable materials. Keywords: Brinkman number or viscosity ratio; Newtonian fluid; mass transfer, Darcy number

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Non-Linear Mixing Dynamics of Viscously and Gravitationally Unstable Flow In Porous Media

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Viscous and gravitational fingering refer to flow instabilities in porous media, which are respectively triggered by adverse mobility or density ratios. Fluid mixing and its interplay with fingering as well as flow channeling through heterogeneous media have received much less attention in compositional and compressible flow. Many important subsurface processes such as CO2 geological sequestration and enhanced oil recovery involve strong species exchange within single or multi-phase fluid systems. Importantly, phase behavior can change local fluid properties, which can either enhance or mitigate flow instabilities, thereby significantly controlling the mixing dynamics. We perform accurate numerical simulations that are thermodynamically consistent to capture fingering patterns and complex phase behavior of mixtures. We present a detailed study of mixing in presence of viscous and gravitational fingering in compositional single- and multi-phase flow. Homogeneous and heterogeneous porous media in two and three dimensions are considered. In particular, we investigate different boundary conditions in density-driven convection, such as Rayleigh-Taylor and Rayleigh–Bénard mixing, for the first time, in partially miscible systems. Universal scaling relations for dispersion and mixing rate are also presented. Second, we uncover non-linear mixing dynamics of a finite-size slug of a less viscous fluid attenuated by a carrier fluid during rectilinear displacement. The results provide a broad perspective into how compositional flow can alter fluid mixing in porous media.

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Optimization of productivity index of a horizontal well with friction loss along the wellbore in a closed rectangular drainage

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In this paper, A new general mathematical model for horizontal well with both laminar and turbulent flow was developed. Coupling this model with reservoir model in a closed rectangular drainage area, the dimensionless productivity index (JD) of horizontal well with friction loss can be obtained. It is shown that the value of JD depends on the interaction of horizontal-well conductivity (ChD), penetration ratio (Ix) and Reynolds number (NRet). In addition, the influences of the production rate q, wellbore diameter (2rw) and the length of horizontal well (Lh) on the productivity index (J) have been revealed. Results show that the production rate q (through NRet) has a negative effect on the productivity index (J) for long horizontal well while wellbore diameter exerts a positive effect on the productivity index (J). The length of horizontal well (Lh) has both positive and negative effect on the productivity index (J). Based on the productivity index (J) or productivity index per feet (Jpf), a new method for optimization of the production rate, length of horizontal well and wellbore diameter was presented. Once two parameters are fixed, we can obtain the optimum value of the third parameter by finding the inflection point on the curves. Our work provides a deep insight for flow mechanism of horizontal well with friction loss in a in a closed rectangular drainage area and proposes a powerful tool for parameter optimization in the field.

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Time adaptivity for Non-Linear Reactive Transport in heterogeneous porous media

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Numerical simulation of reactive, flow and transport in porous media requires that the increasingly non-linear models be solved in an accurate and computationally efficient manner. However, the time step sizes associated with each of these processes differ greatly. For example, kinetic reaction rates varying over order of magnitudes or layered reservoirs with fast and slow concentration changes in high and low permeability layers, respectively. A few texts can be found in literature to address this area: Mortar element technique in both space and time domain , Two-ways methods (Offline/Online) ,Optimized Schwarz waveform relaxation (OSWR) method. We present an adaptive time-stepping approach with different time-step sizes in different spatial domains. In summary, we proposed a mass conservative, adaptive time-stepping scheme with different time step sizes in different spatial domains, a fully implicit solution algorithm was developed for coupled flow and transport problems, using block Jacobi for improved convergence rates, numerical results using DG0 in time and RT0 Mixed FEM in space (finite difference), and preliminary results are in good agreement with reduced error in the fine time domain.

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A large deformation poro-elasto-plastic model for modelling sand production during gas production from methane hydrate reservoirs

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Natural gas hydrate reservoirs are deemed a promising future energy resource. It is widely believed that the energy content of methane occurring in the form of hydrates possibly exceeds the combined energy content of all other conventional fossil fuels (Piñero 2013).

A lot of research effort has been focused towards developing techniques for producing methane gas from these reservoirs. Several methods have been proposed for gas production, which include thermal stimulation, depressurization, and chemical activation (Moridis et al. 2009, 2011). Among these, depressurization is currently considered as the most mature approach. Recently, field trials were conducted onshore in the Alaskan permafrost (Anderson et al. 2014) and offshore Japan in the Nankai Trough (Yamamoto 2013) for evaluating the potential for using depressurization as the essential driving force for releasing gas from natural gas hydrate reservoirs. In these field trials, the uncontrolled production of sand and fine particles emerged as one of the most serious flow assurance and well-bore stability issues with regard to the field applicability of the depressurization method. The production of sands and fines is detrimental to the productivity of the production wells as it significantly increases the maintenance and the operational costs.

To design effective sand control methods, it is imperative to develop modeling approaches that predict the sand flow and production behavior in relation to the production conditions.

Here we present a mathematical model and numerical solution strategy for coupled thermo-chemo-hydro-geomechanical processes occurring in natural gas hydrate reservoirs. We focus on the gas production application, and account for gas hydrate reaction kinetics; non-isothermal multi-phase, multi-component flow; and mechanical deformation of the sediment. To model the sand flow, we cast the problem in a large deformation poro-elasto-plasticity framework.

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Effect of Spinal Cord Porosity in relation to Syringomyelia

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Syringomyelia is a disease where fluid filled cysts or “syringes” within the spinal cord develops over time. The disease is often seen together with the Chiari Malformation I (CMI), which is a downwards displacement of the cerebellar tonsils into the subarachnoid space (SAS) where cerebrospinal fluid (CSF) flows. Partial block of CSF flow affects the pressure environment as well as fluid flow in the SAS along the spinal cord. Many theories have been proposed to explain the link between CMI and syringomyelia [1], but have not been validated.

Most research on modeling the spinal cord has focused on Computational Fluid Dynamics (CFD) or Fluid-Structure Interaction (FSI). Some of the theories explaining why a syrinx expands, rely on a pressure difference between the syrinx and the SAS followed by a bulk flow into the syrinx. A poroelastic representation allowing fluid flow within the cord, has the potential to increase our understanding of why bulk flow into the syrinx occur.

In our study, an idealized model of the spinal cord an SAS is constructed consisting of the C1-C6 segments of the region. The 2D model consists of an elastic spinal cord surrounded by the SAS containing CSF (Figure 1). The governing equations in the SAS and inside the syrinx are the incompressible Navier-Stokes equations, while linear poroelasticity is used in the spinal cord. On the interface between the spinal cord and SAS, continuity of stress and velocities are assumed, and the dura mater (outer walls) is assumed rigid. In the model, a pressure difference between the fluid inlet and outlet is imposed. This difference is either sinusoidal, or based on pressure measurements (measured by Friĉ and Eide). For the elastic cord, we assumed no displacements at the top and bottom. The equations are solved simultaneously in FEniCS with a monolithic finite element method using Eulerian coordinates on a moving domain. A similar model using an elastic spinal cord is also made for comparison. More detail on both models are given in [2]. To investigate different factors behind progression of the syrinx, we also vary the syrinx diameter and cord stiffness (Young's Modulus, E).

Our studies show that a sinusoidally varying pressure difference with amplitude 20 kPa, results in CSF flow up to 6 cm/s in the SAS and causes the syrinx velocity to be 180 degrees out of phase with CSF velocities in the SAS (Figure 2). Furthermore, a sharper pressure wave causes higher syrinx velocities. Poroelastic properties of the cord cause both delay and damping to the traveling wave within the cord compared to an elastic cord. This in turn causes lower fluid velocities within the syrinx (Figure. 3).

Inertial waves inside the syrinx may be a possible cause of damage to spinal cord tissue, especially with higher velocity fluid flow and steeper pressure waves. Porous effects contribute to damping of the system. The next step in our work is to evaluate bulk flow into (or out from) the syrinx for the different cases.

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Linearization techniques for non-linear Biot's model

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Coupled flow and geomechanics models have several applications including CO 2 sequestration, geothermal energy, and subsidence phenomena. Biot's model is often used for describing this coupled behaviour. The development of robust, efficient and accurate numerical methods to solve Biot's model has recently attracted a lot of attention. In particular, splitting techniques that decouple the flow and mechanics problems, have been proposed and analysed [1, 2]. So far, the rigorous analysis of the convergence of the splitting techniques has been obtained only for the linear problems (both flow and mechanics).

In this work, we propose new schemes for solving the non-linear Biot model. The schemes are analized rigorously. More specifically, we consider the case when the Bulk modulus (Lame coefficient λ) and the fluid compressibility are non-linear satisfying certain structural conditions. We compare the performance of the splitting scheme against a monolithic scheme and it shows similar CPU time. For a fair comparison, a block preconditioner is used to solve the algebraic system obtained by the monolithic scheme. The block preconditioner used exploits the block structure of the linear system obtained by the proposed splitting scheme. We discretize in space by using MFEM for the flow and Galerkin FE for the mechanics. The backward Euler method is used for the temporal discretization. The convergence analysis uses the techniques developed in [3, 4, 5], namely showing that the scheme is a contraction in appropriate norms thereby also providing the convergence rates.

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Nonlinear elasto-plasticity for Earth's lithosphere extension

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The objective of this work is the numerical simulation of the Earth's lithosphere extension that is a tectonical process which possesses a deep influence on other geodynamical phenomena and on the spatial distribution of some important natural resources. During last decades a large amount of research concerning this topic has been performed by means of analogical and numerical models, named sandboxes. This work is motivated by the observation of several issues inherent to the analogic experiments and by the generally accepted adoption, in the known literature, of purely linear rheologies for numerical tests, which are clearly incoherent with the natural finite-strain deformation regime of the problem at hand. In this work a fully-nonlinear elasto-plastic rheological approach has been developed and implemented. The variables of the problem are parametrized by material coordinates thus a totally-Lagrangian formulation has been adopted; furthermore the analysis of the dimensionless quantities of the governing equations justifies the assumption of a quasi-static motion. In order to avoid the volumetric locking arising from the local strong enforcement of a nearly incompressible deformation, a three-fields weak variational formulation of the problem has been taken into account, as discussed in [Simo1998]: this method consists in the weak enforcement of the volumetric constraint by means of a new independent dilatation variable. Coherently to the fully-nonlinear rheological approach the deformation gradient is multiplicatively decomposed according to the Kroner-Lee decomposition. The global nonlinear system is solved by application of the Newton-Raphson linearization method. The constitutive update, which is computed point-wise on the quadrature nodes, is carried out firstly determining an elastic trial state; if the trial state is nonadmissible, the exponential return map algorithm is performed in order to recover admissibility. The nonlinear return map scheme is solved by means of the Newton-Raphson linearization method. A new C++ MPI-parallel code has been implemented; it is based on the deal.II finite element library; it handles three-dimensional multi-layered domains. The results are encouraging since they show the natural development of V-shaped shear bands which is a deformation pattern that the most-diffused softwares in the geodynamics field are able to catch only if a weak seed is artificially added into the domain.

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NUMERICAL APPROXIMATION OF FLOW THROUGH FRACTURES IN POROELASTIC MEDIA

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We develop a computational model to study the interaction of a free fluid with a poroelastic material. The coupling of Stokes/Brinkman and Biot equations represents a prototype problem for these phenomena, which feature multiple facets. On one hand, it shares common traits with fluid-structure interaction. On the other hand it resembles the Stokes-Darcy coupling. For these reasons, the numerical simulation of the Stokes-Biot coupled system is a challenging task. The need of large memory storage and the difficulty to characterize appropriate solvers and related preconditioners for the equations at hand are typical shortcomings of classical discretization methods applied to this problem, such as the finite element method for spatial discretization and finite differences for time stepping.

We present and thoroughly analyze a loosely coupled scheme for Stokes/Brinkman-Biot coupled equations. The scheme is based on Nitsche's method for enforcing interface conditions. Once the interface operators corresponding to the interface conditions have been defined, time lagging allows us to build up a loosely coupled scheme with good stability properties. The stability of the scheme is guaranteed provided that appropriate stabilization operators are introduced into the variational formulation of each subproblem. The error of the resulting method is also analyzed, showing that splitting the equations pollutes the optimal approximation properties of the underlying discretization schemes. In order to restore good approximation properties, while maintaining the computational efficiency of the loosely coupled approach, we consider the application of the loosely coupled scheme as a preconditioner for the monolithic approach.

We also discuss a topological model reduction strategy in the Stokes/Brinkman region based on volume averaging. In particular, the equations are averaged over the cross-sections, giving rise to a reduced flow model on the fracture midline. We derive suitable interface and closure conditions between the Biot system and the dimensionally reduced Stokes/Brinkman model that guarantee solvability of the resulting coupled problem. We design and analyze a numerical discretization scheme based on finite elements in space and the Backward Euler in time, and perform numerical experiments to compare the behavior of the reduced model to the full-dimensional formulation and study the response of the model with respect to its parameters.

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Numerical simulation of fault re-activation using poroelastic material models

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In some industries, we need to inject fluid into the rock reservior, such as petroleum, geologic storage of carbon dioxide etc. The fluid injection can alter the stress field in the reservoir, which could induce the preexisting fault to reactivate. Our research focuses on this problem and uses eXtended Finite Element Method to develop the numerical method used to analyze the probability of fault reactivation. Thanks to the eXtended Finite Element Method, we can model curved faults. In order to study the slipping behavior of the fault in the process of reactivation, our research uses the zero-thickness interface elements to represent the fault. Besides, we present a reduced model of the fluid flow in the fault so that the zero-thickness interface elements can also account for the variation of the hydraulic aperture and the permeability of the fault in the process of reactivation. We particularly focus on the map-view two-dimensional case, while when considering the dip of the fault, we regard the system as a two-and-one-half dimensional system based on Anderson's fault theory which assumes the vertical direction as principal stress component. We use the Rate- and state- dependent friction model as the fault friction model, and use Biot's theory of poroelasticity to study the coupling between fluid flow and mechanical deformation in porous media. Since the Fully Coupled Method between fluid flow and poromechanics is computationally expensive, we prefer the Iteratively Coupled Method. In particular, we apply the Fixed-stress Split. In such scheme, the fluid flow problem is solved firstly by freezing the total means stress field, and then the results are used to solve the mechanical problem. The Fixed-stress Split is unconditionally stable, consistent and more accurate for a given number of iterations compared with the undrained split. In order to verify our code, we some test cases are presented. For the coupling between fluid flow and poromechanics, we consider the Terzaghi Problem and the Mandel Problem, the results are similar to that in previously published works.

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Visco-elasto-plastic model for Earth crust deformation

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The aim of this work is the numerical simulation of crust deformation processes, motivated by the fact that these geological phenomena play a very relevant role in geodynamics investigations. In this sense a good portion of the research currently done about this topic by scientists consists in the analysis of analogical models, named sandbox, which try to reproduce the real phenomena. The development of a numerical sandbox, that is the objective of this work, is motivated by the several issues inherent to the analogic experiments: they are expensive, they are extremely simplified, their results are mostly qualitative, they they do not account for thermal effects and the gravitational force cannot be rescaled. The constitutive laws that control the motion of the numerical sandbox are described by a fully-nonlinear visco-elasto-plastic rheology which is best suited for finite-strain deformations. The motion is described in a Lagrangian way since the spatial physical quantities that represent the variables of the problem are parametrized on the reference configuration. Thanks to the nondimensionalization of the equations a quasi-static motion is assumed. For the numerical discretization a three-field variational formulation of the problem has been taken into account in order to prevent the volumetric locking arising from the enforcement of a nearly isochoric deformation, as stated in [Simo1998]: an independent volume field is introduced together with its dual variable that can be interpreted as the Kirchhoff pressure. This leads to an additive decomposition of the Helmoltz free energy into its isochoric and volumetric parts. The implicit update of the state of the system is computed by means of the Newton-Raphson method. Using the Kröner-Lee decomposition, the deformation gradient is multiplicatively decomposed into its elastic and plastic parts. The constitutive update is computed point-wise on the spatial quadrature nodes: an elastic trial is firstly computed; if the trial deformation lies outside the elastic domain then the plastic exponential return map brings the nodal deformation back on the boundary of the elastic domain. A Drücker-Prager yield failure criterion and a non-associative flow rule have been considered since these are really good choices for geological applications, as stated in [BelytschkoLiu2001]. The code is written in C++, it is based on the deal.II finite element library, it works in parallel by means of the MPI and multi-threading paradigms, it handles three-dimensional geometries. The results show the natural formation of shear bands with a V-pattern that the most-diffused softwares for geodynamics simulations are able to catch only if a weak seed is artificially added into the domain.

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Abstract submission to Minisymposium 2.6

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Accurate estimation of snowmelt flux is of primary importance for runoff hydrograph prediction for water management and flood forecasting. Lateral flows and preferential flow pathways in porous media have proven critical for improving soil flow models (de Rooij, 2000), but only 1D matrix flow is accounted for in the most sophisticated physically-based snowmelt models. Currently, a single drying water retention curve to estimate capillary pressure within both drying and wetting snowpacks is used. Thus, there is an immediate need to develop snowmelt models that represent lateral and finger flows as well as full capillary hysteresis to examine the potential to improve snowmelt hydrological modelling. A 2D model has been developed that enables an improved understanding of energy and water flows within deep heterogeneous snowpacks on flat and sloping terrains. The numerical model simulates 2D water flow through snow matrix and flow fingers through capillary hysteresis, internal energy fluxes, melt at the surface, and internal refreezing. The wetting boundary curve is scaled from the drying boundary curve (Kool and Parker, 1987) and the scanning curves are estimated using the model presented by Luckner et al. (1989). The dual pathway model utilizes an explicit finite volume method to solve for the energy and water flux equations over an orthogonal grid. Initial snow properties - dry density and grain size - and input water flux at the surface were taken from laboratory data presented in Katsushima et al. (2013); comparisons with their experimental results show that including a wetting boundary curve better represented the capillary overshoot at the interface wet to dry snow, whereas adding the scanning curves improved the simulation of capillary pressure at steady state. Introducing capillary hysteresis impacted the water saturation within the snowpack, as well as the formation of preferential flow paths and their characteristics. Thus, heterogeneous flow models in snow can be useful tools to help understand snowmelt flow processes and how snowmelt-derived streamflow forecasting might be improved.

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An interior penalty discontinuous Galerkin scheme for two phase flow in heterogenous porous media with discontinuous dynamic capillary pressure effects

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The mathematical models describing flow and transport processes in porous media are, in general, coupled systems of evolution equations. The difficulties associated with such problems arise from their highly non-linear, possibly degenerate character, changing their in type in a manner that is not known a priori but depending on the model unknowns. Additionally, realistic models are defined in heterogeneous media, with location dependent parameters and non-linearities. Discontinuous Galerkin (dG) methods are well suited to deal with heterogeneous media. First of all, they already include inter-elemental interface conditions, thus including conditions coupling homogeneous porous blocks can be done naturally. Furthermore, dG methods fundamentally provide discontinuous solutions. For heterogeneous porous media, where the saturation and even the phase pressure difference may become discontinuous when passing from one homogeneous block to another [1], dG methods are more suited than continuous Galerkin (cG) ones as the latter provide solutions that are continuous over inter-elemental interfaces, which leads to either oscillations or unnecessarily smeared out profiles. Here we consider a two-phase porous media flow model that includes dynamic effects in the capillary pressure. The medium is heterogeneous, consisting of homogeneous blocks. An Euler implicit - dG method scheme is presented and analyzed [2], with particular attention paid to the coupling conditions imposed at interfaces separating homogeneous blocks. To deal with the nonlinear systems resulting at each time step after applying the space-time discretization, we use a recently developed variation of the Picard method, the L-scheme [3,4]. While primarily a fixed point iteration, the method inherits a global convergence property with only a mild restriction on the time-step as compared to Newton-method.

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Analysis of Dynamic Capillarity Effect in Modeling Saturation Overshoot during Infiltration

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It is known that during downward infiltration of water into dry sand, fingers are formed. Moreover, the water saturation profile within each finger is non-monotonic, with a saturation overshoot at the finger tip. Richards equation cannot simulate the occurrence of fingers and non-monotonic saturation behavior. In this work, we analyze an extended form of Richards equation where dynamic capillarity effect is included. In this model, the pressure difference between two phases is specified to be related to the standard capillary pressure plus a term depending on the time rate of change of saturation. The coefficient of proportionality, denoted by τ, is called the dynamic capillarity coefficient. The coefficient τ controls the extent of saturation overshoot in a finger. Experimental and numerical studies have shown that the value of τ may depend on saturation. Based on reviews of numerical and experimental studies as well as mathematical analysis, we investigated four typical relationships between the coefficient τ and water saturation. We performed traveling wave calculations and compared numerical simulations with a recent water infiltration laboratory experiment. Different functional types were found to have a crucial impact on the saturation profiles.

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Coupling porous-medium and free-flow systems: alternative model formulation and validation

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Classical concepts for porous-medium and free-flow systems include coupling conditions at the sharp interface between two systems, which cannot store and transport mass, momentum and energy. These concepts are restricted to flat interfaces and flows nearly parallel to the interface, which is not the case e.g. for filtration problems. Recently, a coupling concept for flows perpendicular to the interface is developed using homogenization. However, a general model formulation is still missing.

In this talk, an alternative coupling concept which is suitable to arbitrary flow direction and allows transport of thermodynamic properties along the interface will be presented, where free-flow and porous-medium systems are coupled via a non-simple interface (transition region). The closed model consists of the Stokes equations in the free-flow domain, Darcy's law in the porous medium and the transition region model describing flow dynamics of the non-simple interface. The proposed coupling concept is validated by direct numerical simulations and compared to the classical interface conditions.

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Determining the mobile water content of a non-saturated porous material with a fractional advection diffusion equation

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Several experimental methods record the water content of non-saturated porous materials, but it often happens that part of the wetting fluid is trapped, and we do not know how to measure the corresponding volumic fluid fraction. Nevertheless, some mass transport models account for mobile and immobile fluid fractions qm and qim . They are schematized by partial differential equations (pdes) whose coefficients depend on these quantities, which often are spatially non-homogeneous. On the basis of such pde we deduce qm and qim from series of concentration profiles. Indeed, efficient optimization methods give us the coefficients which minimize the deviation between data and pde solutions.

We demonstrate this within the framework of the fractal variant of the Mobile/Immobile Model (MIM) [1]. The classical variant assumes solute transport ruled by Fick's law applied to the mobile solute concentration (in the mobile fluid fraction), and exchanges with the immobile fraction described by first order kinetics. The latter assumption is equivalent to immobile and mobile concentrations related by a convolution of exponential kernel. The fractal MIM (fMIM) just replaces the exponential kernel by a decreasing power of time [2,3]. It is equivalent to a generalized Advection Diffusion Equation equipped of a supplementary time derivative whose order is not an integer. Our demonstration starts from time concentration profiles recorded (by dichromatic X ray spectrometry) at several cross-sections of a column filled of unsaturated sand in which a passive tracer is injected while the Darcy velocity is steady. Some of these profiles are represented by symbols on Fig. 1. The water content is measured also (see the squares of Fig. 2), and found steady. Yet it strongly depends on space, and this suggests mobile and immobile water contents qm and qim also spatially non-homogeneous. Accounting for these possible spatial variations necessitates supplementary degrees of freedom in the fractal MIM : in addition to the diffusivity and the order of the supplementary derivative, they are the interpolation values of the coefficients related to qm and qim . In our case the shape of the measured total water content profile suggests about sixty degrees of freedom. We estimate these parameters by minimizing the squared deviation between fractal MIM solutions and data along a pathway made of a number of successive steps (here more than 1000) in parameters space : each next step is deduced from the gradient of the squared deviation. Solving one adjoint equation provides this gradient at the price of some algebra necessitating much less computing time. For comparison, finite differences would necessitate solving the fractal MIM as many times as we have degrees of freedom (here sixty) at each step ! The adjoint equation makes it feasible [4] to find estimated parameters, and solving the fractal MIM equipped of them yields computed tracer concentration represented by solid lines on Fig. 1. The nice fit to the data suggests mobile and immobile fluid fractions qm and qim represented by the red and green dashed lines of Fig. 2.

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Mechanics of the liquid-liquid interface under two-phase immiscible flows in porous media

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Flow of the two liquids in a porous medium is associated with propagation of the interface between the liquids. This is not only a moving geometric boundary, but also an active participant of the flow. Physical and chemical phenomena around the moving interface are determining for several processes within groundwater flow, ecology, petroleum engineering, carbon dioxide sequestration. In the petroleum engineering, motion of the interface is a determining factor in waterflooding and different methods of enhanced oil recovery: surfactant flooding, microbial EOR, methods based on mobilization and relocation of reservoir fines (smart waterflooding). The interface between carbon dioxide and brine propagates during carbon dioxide sequestration. The traditional models of two-phase flows (like the Buckley-Leverett model) do not account for the interface between the flowing phases. The recent advanced models for two-phase flow, still, do not account for the interface explicitly. We have derived a new system of flow equations generalizing the classical Buckley-Leverett model, and accounting explicitly for the motion of the interface. Representation of the interface is mechanistic, that is, it is averaged on the macro-scale. The pore-scale details of the motion are not taken into account. However, the force interaction of the phases via the interface is accounted for. As a result, we have obtained a complete closed system of flow equations accounting for the propagation of the liquid-liquid interface. The constituting dependences in this system have been derived on the basis of the simplified models of the phase distribution on the microlevel. The system of equations has been generalized onto the 3D case. A numerical IMPES-type method for solution of the system has been developed. It has been shown that the separating surface is, on average, inclined to the direction of the flow, even for the case of one-dimensional co-current flow. For the steady-state flows, dependence of the relative permeabilities on the relative velocities of the flowing phases has been analyzed and compared to the available experimental data. For unsteady flows, the results of computations show much sharper displacement fronts and more piston-like displacement than predicted by the classical Buckley-Leverett scheme accounting for capillary pressure, even if the value of capillary pressure is rather large. This effect is produced by friction of the flowing phases and their force interaction via the moving inclined interface. Relative contributions to this effect of the different factors (the degree of the phase mixing; the viscosity ratio; the relative size of the interaface; the capillary-viscous ratio) have been analyzed.

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NUMERICAL SIMULATION of RAINFALL-INDUCED LANDSLIDES CONSIDERING HYSTERESIS and SCANNING SOIL-WATER CHARACTERISTIC CURVES

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Rainfall triggered landslides are common threat in many regions of the world and cause loss of lives and properties. The infinite slope model is generally used to simulate the seepage of the rain water into the unsaturated soil slope and to carry out the stability analyses. This study aims to establish a physically-based numerical model rainfall infiltration and ultimate limit state stability of an unsaturated infinite slope, while considering the effect of wetting-drying hysteresis. However, the proposed relations can also be used in incremental form to predict suction in different frameworks (e.g. elastoplastic models) and other physical problems. The hysteretic nature of soil water characteristic curve (SWCC) is captured assuming the virgin drying and virgin wetting curves (which can be obtained from experiments or various fitting equations in the literature) bound all possible values during transition from one regime to the other (scanning curves). These intermediate branches of the SWCC depend on both direction and point of origin on the suction-water content space. The proposed model is derived from geometry of various scanning curves observed in the literature. It is a power-type interpolation between the point of regime reversal and a “target point”, which is the residual state while drying, and a water content value interpolated between the values that correspond to zero suction while wetting. The power parameter in the relations appears to depend on various other properties, such as direction and material. However, variation of the power parameter only marginally changes the shape of the generated scanning curves, which means the model can be simplified by assuming a constant average value for this parameter. This consideration is based on limited amount of published experimental data and needs further understanding and experimental studies. The incremental form of Darcy’s equation was used to evaluate water flow within the infinite slope in case of both infiltration and evaporation. The mass conservation principle was included in the calculations by developing a water distribution algorithm, which ensures the spatial variation of the water content within the infinite slope is always physically possible and prevents the values of water contents out of the bounds (e.g. residuel water content or saturated water content).

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Process-dependent transport through porous media

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Heat and mass transport through porous media is governed by the advection-dispersion equation. Near the forward moving mixing front the longitudinal and transversal dispersion lengths are non-zero. Arguments can be given why in steady transport the dispersion lengths are equal to zero. Although in conventional models the dispersion lengths may be a function of position and time, they are assumed to be process-independent. To 'interpolate' between the time-dependent moving front model and the steady transport model we propose process-dependent dispersion lengths. Near the forward moving front the resulting advection-dispersion equation is equal to the well-established conventional transport model with process-independent dispersion lengths that correctly represents the mixing. However, further behind the moving front, where the mass transport has become (almost) steady, the process-dependent model results in vanishing dispersion lengths and, consequently, in a substantially smaller transverse mixing zone.

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Transitions and tipping points in steady-state two-phase flow in pore networks – Justification based on interstitial flow structure mutations.

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In general, macroscopic two-phase flows in porous media form mixtures of connected- and disconnected-oil flows. The latter are classified as oil ganglion dynamics and drop traffic flow, depending on the characteristic size of the constituent fluidic elements of the nonwetting phase, namely, ganglia and droplets. These flow modes have been systematically observed during flow within model pore networks as well as in real porous media. The volume fractions they occupy within the pore network, depend on the flow conditions and on the physicochemical, size and network configuration of the system (fluids and porous medium). Extensive simulations implementing the DeProF mechanistic model for steady-state immiscible two-phase flow in typical 3D model pore networks have been carried out to derive maps describing the dependence of the flow structure on capillary number, Ca, and flowrate ratio, r. The simulations span 5 orders of magnitude in Ca and r. Systems with various viscosity ratios and intermediate wetting have been examined. The presentation will focus on transitions observed in the predicted behavior of steady-state flows. These systematic transitions can be identified by evaluating macroscopic flow quantities, (e.g. reduced pressure gradient, relative permeabilities, optimum efficiency flowrate ratios), for different flow conditions. Certain critical tipping points over narrow regions of flow conditions are identified as well. These observations are explained by examining the inherent flow mechanisms affecting the structure of the interstitial flows. Implementation of the DeProF algorithm, produced key bulk and interfacial physical quantities, fully describing the interstitial flow structure: ganglion size and ganglion velocity distributions, fractions of mobilized/stranded oil, specific surface area of oil/water interfaces, velocity and volume fractions of mobilized and stranded interfaces, oil fragmentation, etc. Systematic flow structure mutations with changing flow conditions have been identified. Some of them surface-up on the macroscopic scale and can be measured e.g. the reduced pressure gradient. Other remain in latency within the interstitial flow structure e.g. volume fractions or fractional flows of oil through connected-disconnected flows. Deeper within the disconnected-oil flow, the mutations between ganglion dynamics and drop traffic flow prevail. Mutations shift and/or become pronounced with viscosity disparity. They are more evident over variables describing the interstitial transport properties of process than variables describing volume fractions. This characteristic behavior is attributed to the interstitial balance between capillarity and bulk viscosity, depending on the externally imposed flow conditions.

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Traveling wave solutions of Richards equation with gravity for general non-equilibrium capillarity pressure conditions

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The Richards equation is a commonly used model for unsaturated flow through porous media. Two unknowns are involved in the equation: the water saturation and the water pressure. Standard models assume that these are related by a nonlinear relationship determined, again, based on experiments. However, models based on this assumption cannot explain phenomena like saturation overshoot or finger formation, which are observed experimentally [1] but ruled out as solutions to the standard Richards equation [2]. Also, the flow through porous media is hysteretic in nature, but all history dependent effects are disregarded in the standard models [3].

In this work we consider non-standard models, where dynamic and hysteretic effects are included into the pressure-saturation relationship. To understand the behavior of this system, we consider a simplified, one-dimensional case, and study travelling wave (TW) solutions [4]. Their qualitative behavior is discussed first including capillary hysteresis and dynamic capillarity effects separately. Then the general behavior of the system is delineated by incorporating both effects mentioned above. These resulting solutions exhibit non monotone profiles and saturation overshoots, which is in good agreement with the experiments in [1]. Finally, we present a numerical scheme to solve this mathematical model, discuss its convergence, and present some numerical results validating the theoretical findings.

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Evidence of geochemical rock-water interactions during hydraulic fracturing from the analysis of flowback water.

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Shale gas exploitation has known a dramatic increase in the past decade thanks to the development of horizontal drilling technologies and hydraulic fracturing, enabling the exploitation of the hydrocarbon resources trapped in the very low permeability source rocks [1]. Hydraulic fracturing consists in injecting at very high pressure tens of thousands of cubic meters of water, usually containing numerous additives, into the formation, in order to fracture it and increase its permeability. Once the production starts, gas is produced along with very saline water containing heavy metals [2-3-4]. This water cannot be released in the environment without treatments [5] and currently, most of the returned water is recycled to fracture another well, while the rest is injected in deep disposals.

Numerous studies have focused on the reason why the returned water contains so much dissolved salts. The initial hypothesis that the salt comes from halite dissolution has now been set aside and the most widely accepted explanation is that the water used for hydraulic fracturing mixes with the salty formation water initially present in the shale, creating a brine which then returns to the surface via flowback [6]. However, one overlooked phenomenon in the returned water composition is the influence of the water-rock interaction during the residence time of the injected fluid in the formation.

In this study we present a consistent set of data from a real hydraulically fractured well in a shale formation in Alberta. Data were collected on the composition of the flowback water during the first days of production on all major elements and numerous traces, as well as isotope data on oxygen, hydrogen, sulfur, inorganic carbon, lithium and strontium. This set of data shows clearly that the composition of the flowback water follows a two end-members mixing curve for most conservative species, confirming the theory that the salt comes from the mixing of the injected water with the formation water. However, the analysis of this dataset also shows a non-conservative behavior of several species, especially sulfate. Indeed, the sulfate content of the returned water is much higher than what could be expected from the mixing model and most likely comes from the oxidation of pyrite downhole, releasing sulfate, iron and potentially other heavy metals into the returned water. Other evidence of water-rock interaction can be obtained from the behavior of K, Ba among others, showing that the returned water composition is not a simple mixing but involves numerous water-rock interactions. Our research aims then at understanding the coupling between transport, residence time and water-rock interaction during the early stage of hydraulic fracturing and production through the evolution of flowback water composition. Understanding the full chemistry downhole would allow a better tweaking the composition of the water used for fracturing and then help to control in a better way the hydraulic fracturing itself, but also the composition of the returned water, with hopes to lessen the burden of the flowback water treatment.

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Investigation into the effect of confinement and mobility at pore-scale for real rocks

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Multiphase flows in porous media are common in many industrial processes such as oil/gas extraction, and CO2 injection and storage. Therefore, efficient computational tools to analyse the behaviour of such flows are essential to understand and improve these processes. Utilising binary images of porous media, direct simulations can reduce the pre-treatment of complex geometries. With high performance computing techniques, the lattice Boltzmann method offers a numerically efficient approach to simulating these flows. Our new lattice Boltzmann platform is developed to simulate two-phase flows in complex and arbitrary geometries in a reasonable timescale. For instance, a domain of one million of nodes runs in 5 hours on HPC (around 300CPUs) for a 5 million lattice time units. Simulations of single-phase flows in porous media were performed for different configurations. However, studies of two-phase flows at very small characteristic scales (around a micrometre) in a real complex geometry has been scarcely reported in the literature. Moreover, the flows can present different patterns which depend mainly on pore and channel sizes. To investigate this kind of flow, we use the colour-fluid model (Rothman-Keller model), similar to VOF method in the Navier-Stokes solvers. This model includes two steps: a perturbation operator from the classical continuum approach as in VOF (BrackBill force [1]) and a recolouring operator [2]. Interpolation techniques are employed to estimate the real contact angle on curved boundaries and to remove unphysical behaviour [3]. In the Berea sandstones (Figure 1) the porosity is around 0.32 and the ratio between the biggest pore to the smallest channel is more than 20. We can observe some creeping flows due to the contact angle in small channels, and bond percolations and droplet formations in pores. We also perform simulations in a random geometry (figure 2) with a porosity of 0.8. The contact angle plays an insignificant role for the behaviour of the two-phase flow and we obtain bond percolations and droplet formations as in pores of Berea sandstones. Our solver is validated for a large range of mobility (1 to 1000) on static droplets, droplet deformation under a simple shear with confinement, breakup with confinement, two-phase Poiseuille flows and two-phase T-junctions (droplet generations). We are, at present, investigating the effect of the confinement of droplets and the mobility on the Enhanced Oil Recovery (EOR) based on the results from our validations.

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Molecular simulations of transport and separation of gas through nanoporous materials: from toy models to kerogen molecular models

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Fluid transport through disordered nanoporous carbon-based materials is inherent to several applications, namely, hydrocarbon production from coals and shale reservoirs, CO2 sequestration and separation processes by means of carbon-based membranes. The understanding of fluid transport properties in such materials, especially their dependence on thermodynamic conditions and structural properties of the materials, is of crucial importance for the aforementioned applications.

In shale reservoirs hydrocarbons are mostly stored in kerogen, which refers to amorphous organic nanoporous structures found in the source rock. Such kerogen nodules generally stand for less than 5% of the weight content of the shale and are finely dispersed in the mineral matrix of the rock. As a result, the extraction of the kerogen phase results in a powder-like material, which prevents from devising permeation experiments able to capture in-situ reservoir conditions.

In the first part of this work, we therefore use molecular simulations to document the phenomenology of fluid transport and separation through kerogen. In the more general field of carbon membranes, Botan et al. successfully employed the same technique to reproduce some typical features of the experimental results found in the literature [1]. Following the same approach, we investigate the permeation of supercritical fluids through molecular models of kerogen (graph1) developed in our group by means of molecular simulations [2]. More specifically, we characterize the transport coefficients and separation rates of CH4/CO2 mixtures flowing through kerogen membranes under a wide range of thermodynamic conditions. A specific attention is paid to the influence of the porous structure of the different kerogen models on the overall transport properties.

In order to better understand the link between the nanostructure of kerogen and its transport properties, the second part of this work investigates a simpler system (graph2) that captures one crucial feature of the complex amorphous carbon membranes: the steric effect inherent to nanoporous constrictions. As a first approach, we study a molecular model that consists in a monoatomic thick sheet connecting two independent fluid reservoirs via a nanoporous slit. We report how permeation rates depend on several parameters, such as the size of the slit, thermodynamic conditions and the amplitude of molecular interactions. By means of simple theoretical models that reproduce our simulations data, we shed light on the range of mechanisms that rule molecular permeation through nanoporous constrictions.

Upon comparing the results obtained with both systems (kerogen models and nanoporous sheet), we shed light on the molecular sieving and selective adsorption mechanisms and their dependence on the porous structure, which greatly impact the transport and separation of the fluid through the kerogen membrane.

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Multi-scale Equation of State Computations for Confined Fluids

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Fluid properties of five binary mixtures relevant to shale gas and light tight oil in confined nano-channels are studied. Canonical (NVT) Monte Carlo simulations are used to determine internal energies of departure of pure fluids using the RASPA software system (Dubbeldam et al., 2015). The linear mixing rule proposed by Lucia et al. (2012) is used to determine internal energies of departure for mixtures, UDM, in confined spaces and compared to UDM from direct NVT Monte Carlo simulation. The sensitivity of the mixture energy parameter, aM, for the Gibbs-Helmholtz constrained (GHC) equation, confined fluid molar volume, VM, and bubble point pressure are studied as a function of uncertainty in UDM. Results show that the sensitivity of confined fluid molar volume to 5% uncertainty in UDM is less than 1% and that the GHC equation predicts physically meaningful reductions in bubble point pressure for light tight oils.

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Multi-scale representation of gas flow in shale formations

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Hydraulically fractured nano-porous shale is known to feature a complex set of structures, ranging from networks of hydraulically induced fractures at different scales to the natural fractures (connected or isolated) within the fragmented matrix block. These complex structures have been increasingly recognized to play an important role in the production of unconventional shale gas. In this work, we combine a bundle of dual-tubes model with the discrete fracture model for accurate description of flow dynamic in shale systems. The flow in a shale gas matrix is modeled by a bundle of dual tubes model where multiple transport mechanisms are considered, and a nonlinear diffusion coefficient is used to describe the combined effect of molecular diffusion and Knudsen diffusion at nanoscale. Using these capabilities, we study and demonstrate the importance of explicit resolution of different sub-scale structures and their effect on flow dynamics. The performance of the method is tested on different realistic configurations of fractured systems, where various parameters of fracture network are examined. Computational requirements are further improved as we employ the Minisymposium R upscaling technique on field scale problems. The flexibility of the implementation allows us to bring additional degrees of complexity and solve more challenging problems with a multiphase flow in shale formulations.

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Pore-scale processes and time scales determining field-scale production

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Hydrocarbon production from shale formations is dictated by the peculiar mechanisms that characterize transport through low permeability porous media (which can be quite different from viscous dominated flow that takes place in the larger pores of more permeable materials) and by the complex fracture networks that result from hydraulic fracturing. We examine in details how the dominant processes may vary with the pore size (and in particular with Knudsen number) and with reservoir conditions. We show that they can be described by a nonlinear diffusion (or permeability) coefficient that depends on a single parameter. We also discuss the role played by fractures of different size in enhancing the recovery and we show how, under appropriate assumptions, this information can be incorporate in very simple models (such as the Bundle of Dual Tube Model, BDTM, Lunati and Lee, 2014 [1]). We further explore the potential role of adsorption and geomechanics. Finally, we illustrate potential advantages and disadvantages of simple models as compared with more complex representations of the geological reality.

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Production from tight reservoirs – potential application of existing molecular simulation techniques

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The purpose of our presentation is first to review the known aspects of fluid distribution and transport at the nanoscale in tight reservoirs and then to outline which molecular simulation tools are available to perform relevant simulations for production. The high specific surface area of tight gas reservoirs and shales, due to the presence of clay minerals and other fine-grained solids, is such that fluid-rock interactions cannot be neglected for understanding fluid dynamics in its porosity. Classical fluid phase equilibrium concepts and models must be adapted to account for the presence of fluid-fluid, fluid-solid and solid-solid interfaces in these rocks. Classical wetting models based on macroscopic contact angles are unable to predict the influence of fluid chemistry and mineral surface chemistry on fluid retention in the cases of strong wetting that are frequent in practice. The structure of the sedimentary organic matter is also important in organic-rich shales as it is made of kerogen, asphalt-like soluble compounds and light hydrocarbons, with pore size distributions extending as low as 1 nm. Finally, rock deformation under stress through pressure solution is also likely to play a role in compaction, creep and subsidence. The review of existing tools shows that in order to model realistic mineral-fluid interfaces, quantum chemistry at the DFT level is a versatile tool that helps to understand bonding mechanisms of molecules on surfaces and their vibrational properties, and also to provide elasticity constants as well as thermodynamic properties for solids. Furthermore, modeling at this level furnishes useful data for forcefield parametrization. These allow to simulate the adsorption of multicomponent gases on solid surfaces in high pressure conditions using either Monte Carlo simulation or molecular dynamics, and analyze its dependency on geometry (e.g. pore restrictions). Also, forcefield-based models are useful to address the free energy of wetting when liquid structure plays an important role, as is generally the case with injected water. A last aspect that can be addressed with existing molecular simulation techniques is the properties of liquid and vapor phases near interfaces of small radius of curvature or near solid surfaces. Some properties – such as chemical potential or partition coefficients - are expected to vary substantially compared with those of bulk fluids. These effects may be significant in various diffusion processes (Oswald ripening, pressure solution) which are relevant at higher scales (two-phase fluid flow, compaction). We conclude that molecular modelling can certainly provide missing links between the discrete description of matter at the nanoscale and the continuum models required by engineers at the reservoir scale.

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Reservoir Simulation Study for a Tight Natural Fracture and Compositional System – Pauto field Case

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Pauto field is located in Colombia in Piedemonte License. This field has been identified as a low porosity and naturally fractured reservoir with a compositional grading behaviour which generates a rich gas condensate cap in the top and a volatile oil leg in the bottom in some of the compartments of the field.

The Full Field Model section describes the construction of the Dual Porosity/Dual Permeability (DPDP) model using measured data with the history matching of a single porosity (SP) model and its conversion into a DPDP model which was performed in commercial software.

A successful easy reservoir simulation construction workflow theory and application to build a DPDP reservoir model was implemented allowing the estimation of shape factors that are consistent with the initial excess permeability and fracture spacing by adjusting the apparent aperture and fracture intensity by knowing the matrix permeability.

Generally the aperture is generated stochastically in geo-statistical models, but the approximation proposed in this study ties all the variables to keep consistency with the KH from logs and Pressure Build Ups.

Results showed that production and pressure match between the SP and DPDP where very close, it was observed 3 main differences in the modeling: 1) a big difference in the vertical condensate segregation (higher in the fracture system) and 2) a similar reduction in the mobility of oil generated in the matrix system and the SP model and 3) a lower oil and gas restriction to flow in the fracture system which helps to improve the bottom hole pressure of some wells and the water production in some sheets.

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A framework to create a new class of pore-network models without pore shape simplifications

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Pore-network models were found useful in describing important flow and transport mechanisms and in predicting flow properties of different porous media relevant to numerous fundamental and industrial applications. Pore-networks provide very fast computational framework and permit simulations on large volumes of pores. This is possible due to significant pore space simplifications and linear/exponential relationships between effective properties and geometrical characteristics of the pore elements. To make such relationships work pore-network elements are usually simplified by circular, triangular, square, stars and other simple shapes. However, such assumptions result in inaccurate prediction of transport properties. In this contribution we propose a new pore-network modelling framework without pore shape simplifications. To test this hypothesize we extracted 3292 2D pore element cross-sections from 3D images of sandstone and carbonate obtained using X-ray microtomography. Based on the circularity, convexity and elongation of each pore element we trained neural networks to predict the dimensionless hydraulic conductances. The optimal neural network provides 90% of predictions lying within the 20% error bounds compared against direct numerical simulation results. Our novel approach opens a completely new way to parameterize pore-networks and we oulined future improvements to create a new class of pore-network models without pore shape simplifications. In addition to hydraulic conductance we also discuss capillary entry pressure and menisci conductances during multi-phase flow.

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A model for spontaneous imbibition in porous media with pore shape and tortuosity considered

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Capillary-driven flow of wetting liquids, also noted as spontaneous imbibition, is a ubiquitous natural phenomenon. Researchers have paid great attentions on the imbibition process and mechanism in many fields, such as petroleum engineering, soil physics, polymeric composites and biosciences. However, since the complex microstructure of natural porous media, the imbibition properties have not been well understood. By including a uniform pore shape factor, we modify the classical Hagen-Poiseuille equation and Laplace-Young equation. Based on the assumption of capillary tube model, an analytical spontaneous imbibition model is developed for analyzing the effects of pore shape and streamline tortuosity. The new imbibition model is sufficiently general that it subsumes other available imbibition formulations as special cases, such as Handy model, Benavente model, Li and Horne model, Fries and Dreyer model, Aronofsky Model and Cai fractal model. The presented model is tested using available published data for spontaneous imbibition measured in various natural and engineered materials including different rocks, fibrous media, and silica glass.

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Capillary entry conditions for pore cross-sections with arbitrary geometry and wettability

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Multi-phase flow pore-network models critically depend on accurate calculation of capillary entry pressures, when simulating capillary pressure and relative permeability functions. Known for decades, the Minisymposium -P theory has been widely applied to derive analytical expressions for the entry conditions of idealised pore cross-sectional geometries, such as triangle, square, and n-corner star, with simple wettability distributions. The present study extends the application of the Minisymposium -P theory to a new semi-analytical algorithm to estimate capillary entry conditions for pore cross-sections with arbitrary geometry, as directly obtained from 3D microCT pore space images, and wettability. The algorithm carries out fast evaluation of alternative fluid meniscus configurations in the pore cross-sections to select the energetically favourable and admissible configuration and the corresponding entry condition. Alternative configurations may include pore corner wetting films, fluid bridges in constrictions and pinned menisci due to abrupt changes in pore wall geometry and wettability. Preliminary results show considerable differences between the newly calculated entry conditions and the conditions derived for the equivalent idealised shapes and wettability. Implementation of the algorithm in a pore-network model further highlights the significance of this development, at limited added computational cost.

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Characterizing CO2 capillary heterogeneity trapping through macroscopic percolation simulation

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Having a better understanding of CO2 trapping behavior is highly important and necessary to ensure long-term stability of CO2 geologic storage. Previous work has shown that millimeter-scale heterogeneity in rocks have significant effects on CO2 plume migration immobilization [1]. In order to accurately predict the amount of CO2 capillary heterogeneity trapping caused by millimeter-scale heterogeneity after injection during the plume migration stage, we are in the process of building a Matlab-based macroscopic percolation simulator that has been tested against some full-physics reservoir simulation and coreflooding experiment results. The objective of this study is to characterize a reservoir rock using the degree and type of heterogeneity to predict its post-spontaneous-imbibition CO2 secondary physical trapping behavior.

The Matlab-based macroscopic percolation simulator works by assigning heterogeneous local-scale (voxel-level) properties and implementing displacement and trapping rules. The local-scale properties include porosity, permeability, and capillary pressure curves. A unique capillary pressure curve is assigned to each grid block through scaling the reference capillary pressure curve by the grid block's permeability and porosity. We model drainage with invasion percolation and imbibition with ordinary percolation, always treating water as the wetting fluid and CO2 as the nonwetting fluid. Grid block sizes are on the millimeter scale so flow is simulated directly at the scale of representative elementary volume, assuming no viscous forces and instant capillary equilibrium.

Three sets of two-dimensional permeability fields were fed as input into the macroscopic percolation simulator to predict the amount of in-situ post-imbibition capillary heterogeneity trapping. The results show that CO2 capillary heterogeneity trapping increases with the degree of subcore-scale heterogeneity (measured by standard deviation of log-permeability), decreases with isotropic correlation length, and remains unchanged with respect to anisotropy. The factor that has the strongest influence on capillary heterogeneity trapping appears to be capillary heterogeneity. The results match well with full-physics reservoir simulation results.

We also conducted CO2/water coreflooding experiment in the capillary-dominated flow regime to explore the relationship between permeability variability and CO2 secondary physical trapping. The previous two-dimensional macroscopic percolation simulation results suggest that CO2 tends to be trapped in higher permeability regions. This characteristic of capillary heterogeneity trapping is also clearly seen in experiment results for Fontainebleau sandstone core but less clearly seen for Berea sandstone core. This result may suggest that capillary heterogeneity trapping is more important compared to snap-off trapping for Fontainebleau than for Berea. Furthermore, Fontainebleau, which is more heterogeneous and more correlated, traps more post-imbibition CO2 in total than Berea.

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Direct Numerical Simulation of capillary dominated flows using the Volume of Fluid method.

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We present a comparative numerical investigation on the precision of several formulations of the Volume of Fluid (VOF) method, for the capillary driven spontaneous imbibition within a two-dimensional tube. Using VOF with the traditional Continuum Surface Force (CSF) formulation fails to provide a consistent velocity field at regions close to the interface for capillary numbers, (Ca) smaller than 0.1. At these low Ca flows, the capillary forces dominate over the viscous forces. The numerical error caused due to the imbalance of capillary forces in the Navier-Stokes equations generate parasitic velocities (also referred to as spurious currents) at the interface. Eliminating parasitic velocities is important as these could result in non-physical interfacial re-configurations. Different VOF formulations exist to address parasitic velocities. Here, we investigate different sharp surface formulations, Sharp Surface Force (SSF), Filtered Surface Force (FSF) as well as the Piecewise Linear Interface Construction (PLIC). SSF helps to capture sharper capillary forces whereas FSF filters parasitic velocities developed parallel to the interface. PLIC reconstructs an infinitely sharp interface using analytic solutions based on the volume fraction of fluids present within a control volume. CSF, SSF and FSF are implemented in the OpenFOAM CFD toolbox whereas PLIC in the Gerris Flow Solver. We validate the results against the analytical solution of Washburn's equation derived from Hagen-Poiseuille's relation that predicts the velocity of the meniscus for different viscosity ratios. We observe that at capillary numbers greater than 3x〖10〗^(-3), we never reach a mesh independent solution due to the stress singularity that develops on the wall surface using a no-slip boundary condition and a static contact angle. At capillary numbers, less than 3x〖10〗^(-3), the magnitude of the stress singularity is low leading to a mesh independent solution. We then quantify the parasitic velocities at regions close to the interface for each formulation and investigate their impact on capillary numbers less than 3x〖10〗^(-3). The magnitude of parasitic velocities are maximal for the CSF formulation and reduces by a factor of two using SSF. Though FSF reduces parasitic velocities considerably, we observe periodical bursts in the velocity that exist for short intervals of time. No parasitic velocities are seen with the PLIC formulation. PLIC can effectively be used to study capillary dominated flow regimes to give us new insights on ganglion dynamics.

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Effects of microstructure on water imbibition in sandstones by using X-ray computed tomography and neutron radiography

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Capillary imbibition in variably-saturated porous media is important in defining displacement processes and transport in the vadose zone and in low permeability barriers and reservoirs. Non-intrusive imaging in real time offers the potential to examine critical impacts of heterogeneity and surface properties imbibition dynamics. Neutron radiography is applied as a powerful imaging tool to observe temporal changes in the spatial distribution of water in porous materials. We analyze water imbibition in both homogeneous and heterogeneous low permeability sandstones. Dynamic observations of the advance of the imbibition front with time are compared with characterizations of microstructure (high resolution X-ray computed tomography), pore size distribution (Mercury Intrusion Porosimetry) and permeability of the contrasting samples. We use an automated method to detect the progress of wetting front with time and link this to square-root-of-time progress. These data are used to estimate the effect of microstructure on water sorptivity from a modified Lucas-Washburn equation. Finally, we use these data to link observed response with the physical characteristics of the contrasting media - homogeneous versus heterogeneous. It is also proved that sorptivity is sensitive to the tortuosity instead of porosity in low permeability sandstones.

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Estimation of sub-core permeability statistical properties from coreflooding data

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A new method for estimating sub-core permeability geometric mean and log-permeability variance is presented. The method is based on matching coreflooding experiment measurements of wetting phase relative permeability with semi-analytical calculations of effective relative permeability. The semi-analytical solution is formulated assuming log-normal permeability (k), steady state and capillary-limit conditions. It is based on the geometric mean and log-phase-permeability variance for isotropic k and power law averaging for anisotropic correlations. The solution is validated on synthetic k realizations by comparison with numerical calculations. Then, the estimation method is tested on synthetic data assuming various types of core capillary pressure relationships, relative permeability functions and k anisotropies. Results demonstrate high accuracy in almost all of the cases except for small anisotropy ratios between horizontal and vertical dimensionless correlation lengths, where flow is in the horizontal direction, and when variance is large. The method is also validated using data from CO2-brine coreflooding experiments conducted on two different cores. It is found that the estimation method remains accurate in these realistic settings, however, accuracy of k geometric mean is reduced when the core permeability departs from a log-normal distribution.

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Experimental Study of the Effect of Adsorbed Layer on Shale Permeability

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Understanding the gas transport and determining the permeability are essential for investigating the gas flow mechanism and evaluating a shale formation. Current methods for measuring permeability and/or diffusivity may lead to erroneous results when applied to gas shale. The effect of adsorbed gas is neglected in modeling flow through conventional rocks. This is reasonable because the volume occupied by adsorbed layer is negligible compared to the total void space in conventional rocks. However, the adsorbed volume of CH4 is crucial in shale because the pores are often smaller than 10 nm and much of the void space is in the organic material, to which CH4 has a large affinity. As a result, the gas permeability of these rocks is affected significantly not only by the pore size distribution, but also by the adsorbed layers on the walls. Since most of the permeability is measured with helium or nitrogen, in which condition the adsorbed layer is not considered when adsorption actually occurs, permeability for a shale reservoir will be underestimated. To better understand the effect of the adsorbed layer on shale permeability, the most straightforward way is to measure the parameter with CH4 by properly designed experiments. It is shown from the test results that the permeability increases with declining pressure. This could be explained that the adsorbed layer diminishes in thickness as the pressure decreases. Moreover, it is found that the permeability increases nonlinearly as the in-situ pressure decreases during production. This effect contributes to mitigate the decline in the production rate of shale-gas wells. The results obtained in this study have implications for measuring shale permeability accurately at laboratory conditions and for interpreting gas flow rates from production wells over time.

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Fractal characterization of rock properties in 3D rock images

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Rock properties, such as porosity, permeability and electrical conductivity, are important parameters for characterizing fluid flow and heat transfer in porous media. One of the statistic approach to estimate these properties is the well know fractal theory, which represents the pore space as a bundle of capillary tube model (BCTM), and the cross section of the tubes are expressed analytically with fractal distribution. Based on BCTM, especially with circular cross section, the rock properties could be expressed analytically, and the pore geometry, wettability effect could then be justified. One main disadvantages of the existing fractal models is that the connectivity is missing, as all the pore space is accessible in a BCTM. In this work, we aim to characterize the rock properties in 3D rock images, which the rock connectivity will be take into consideration. The fractal dimension of a real 3D rock sample is obtained by extending the 2D box counting method to allow for 3D objective. The relationship between the fractal dimension of 3D rock and that from 2D cross section were studied extensively, which suggest that the currently used simple correlation is fail to estimate the fractal dimension in 3D rocks. The pore skeleton is added in the formulation for rock permeability calculation to account for the connectivity. Our simulated permeability from fractal theory is then compared directly with that from pore scale modelling.

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Geometrical and topological characterization of Micro-fractures in coal seams for flow modelling

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Natural micro-fractures in ultra-tight formations, such as shales and coal seams, provide key information about in-situ states of stress, geo-chemical reaction and fluid flow in past and present. By characterising micro-fractures in core samples, in terms of their connectivity, geometry and surface properties, we can therefore develop appropriate models to gain better understanding of the roles of open micro-fractures on the drainage of hydrocarbons from matrix pores and to design field treatments for mineral-filled fractures by forward simulations. In this work, we developed a new characterization method to identify fractures in CT images and to characterize their geometric properties and surface roughness. First we improve the medial surface-based fracture representation by introducing a new set of skeleton points, especially including surface points with Euclidean distance and edge points with connectivity information. Ideal and real fracture models are used to verify our algorithm, and all results show good agreement between the topological structures of the fractures and flow path obtained from flow simulations. By combining Euclidean distance and geometric transformation, the width, orientation, and inclination angle of micro-fractures can be computed. Connectivity information at each and every edge point is obtained to enable the simulation of flow interaction between a fracture and the matrix appropriately. Moreover, as surface roughness could cause methane gas to be trapped in fractures, cross section of the edge points' 26 neighboring voxels was introduced to quantify surface roughness of the micro-fracture. Overall, our new method improves micro-fracture characterization and the accuracy and precision of the pore-space reconstruction for gas flow modelling.

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Modelling Capillary Pressure and Relative Permeability in Dual-Wettability Media

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Recent studies show that the pore network of unconventional tight and shale rocks generally consists of inorganic and organic parts. The organic part is strongly oil-wet and preferentially imbibes the oleic phase. In contrast, the inorganic part is usually hydrophilic and preferentially imbibes the aqueous phase. The conventional theories of capillary pressure and relative permeability which are based on uniform wettability, cannot be applied to model phase positioning and permeability in unconventional rocks with dual-wettability behavior. This presentation will demonstrate how the conventional theories can be modified and extended by combined analysis of comparative imbibition data and mercury injection capillary pressure data.

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Numerical simulation of the steady motion of a non-wetting slug in a microchannel using a Phase-Field model

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We present an extensive analysis of the precision of a Phase-Field Model (PFM) for the capillary driven motion of a non-wetting slug in a two-dimensional microchannel. The thickness of the lubricating films that form on each side of the channel, separating the slug from the walls, is typically two orders of magnitude smaller than the channel width. Hence, capturing this film and resolving the flow inside it is a challenging task. The Volume-Of-Fluid (VOF) method can accurately predict the film thickness when the grid resolution is fine enough, but the velocity obtained suffers from spurious currents. PFM is investigated as an alternative method. The model is based on an energetic variational formulation that couples the Navier–Stokes system with the Cahn–Hilliard equation through an additional stress term and an additional diffusion-compression term in the transport equation. The additional stress term describes the surface tension effect in term of the gradient of a chemical potential, while the diffusion-compression term maintains the phase equilibrium in the interface zone. The results are compared with two VOF methods with sharp formulations that lead to reduced spurious currents. The various methods are implemented in the OpenFOAM CFD toolbox. We observe that PFM gives a more accurate velocity field than VOF. Moreover, the diffusion of the interface does not prevent the formation of the thin films and PFM can predict their thickness as accurately as VOF. Since the velocity field is free of spurious currents, adaptive mesh can be used to improve computational efficiency or thin film thickness accuracy without convergence issues. Thus, PFM could potentially be used to achieve fast and accurate simulations of capillary driven flow on complex 3D geometry.

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Pore scale characterization of unconventional coal bed methane reservoirs

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The study of multiphase flow in porous media is intensively being developed as the result of the recent introduction of new methods of rock analysis. Invention of modern rock properties measurements techniques which made possible to analyse the structure of rocks on the pore scale leads to thorough understanding of two-phase displacements in reservoir rock. The latter is particularly important for unconventional reservoirs such as shale oil, shale gas, coal seam gas and tough carbonates. Coal seam gas (CSG), also known as coal bed methane (CBM), is a form of unconventional natural gas extracted from coal reservoirs. Coal seam gas reservoirs are unconventional in the sense that the scale of vertical and lateral variability is high when compared to conventional sandstone reservoirs. This requires higher resolution data (sub-microns level) for calculation of reservoir properties and multiphase flow simulation. This project has two main aims. The first one is to perform micro-CT scanning and obtain high-resolution images of coal samples which will be processed, filtered and segmented to pore space and matrix matter. This will allow us to extract the pore system of the coal, which is typical multiscale, cleat-macro-micro, pore system. It is planned to use SEM data for validation of the results. The second aim is to exploit the segmented images to simulate multiphase flow in the pore space of coal. The result of multiphase flow will enhance our understanding of the behaviour of the fluid in the coal seam gas reservoir at pore scale. The simulated coal properties, such as porosity and permeability, will be compared to MICP data for validation.

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Pore scale numerical simulation of spontaneous infiltration in tight porous media

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In recent decades, spontaneous imbibition in porous media has received much attention in a wide variety of fields. Many theoretical and analytical models for spontaneous imbibition of porous media were proposed for many years. However, most of them barely dealt with the internal geometry or microstructures beyond very simple geometrical arrangements, in spite of the critical importance of those factors on the spontaneous imbibition of porous media. At the nanometer scale, the spontaneous imbibition in tight porous media will be more affected by the structure and shape of the pores. Given the limited power of the existing theoretical models in dealing with porous media, the numerical methods are becoming increasingly important and more widely used in the porous media. A complete numerical determination of the spontaneous imbibition of porous media has to include such two major steps as first reproduced by a random generation-growth algorithm, and then the corresponding transport governing equations are solved using a high-efficiency lattice Boltzmann method. This methodology can also be extended to other transport of porous media.

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Pore-scale simulation of three-phase gas and water invasion processes on 3D rock images

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Understanding multiphase flow in porous media, including the mechanisms for mobilization and trapping of isolated fluid ganglia, is important for recovery and storage applications in mature hydrocarbon reservoirs. We use a new multiphase level set (MLS) technology [1] to simulate quasi-static, capillary-dominated gas and water invasions after two-phase imbibition processes, directly on segmented 3-D rock images. We investigate three-phase capillary pressure and hysteresis behavior, as well as the double displacement mechanisms involved during three-phase gas and water invasion cycles that reduces residual oil saturation further from that after a two-phase water flood. We include structured adaptive mesh refinement (AMR) and run large parallel simulations using the national high-performance computing e-infrastructure. We show that AMR improves accuracy of oil layers surrounded by gas and water in pore corners, and it has an effect on calculated macroscale properties, such as specific interfacial area, as well. The MLS method accounts for arbitrary wetting states and volume preservation of isolated fluid ganglia that may coalesce or split. We simulate three-phase capillary pressure-controlled experiments, to imitate standard capillary-pressure measurement techniques in core samples, and three-phase saturation-controlled experiments, to imitate experiments controlled by (constant) flow rate. Many two-phase pore-scale flow experiments have shown that the latter type gives rise to co-operative behavior. Based on simulations, we show co-operative behavior during three-phase displacement in porous rock and demonstrate that, the saturation paths, structure of residual oil, interfacial area, capillary pressure curves and hysteresis behavior, all are different when compared to similar three-phase capillary pressure-controlled experiments. These findings highlight the importance of carefully designing pore- and core-scale experiments that capture the desired boundary conditions and flow conditions.

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Pressure Transient Analysis in Low Permeability Reservoir with Pseudo Threshold Pressure Gradient

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The implementation of a welltesting program of buildup tests conducted on wells in low permeability reservoirs has revealed a unique and consistent characteristic of the pressure transient response. The characteristic is that pressure change and pressure derivative curves exhibit a straight line of slope larger than zero after radial flow regime. The test pressure responses cannot be interpreted by a composite reservoir model because a composite reservoir model should not exist for every well in a reservoir with very small water cut that is less than 1%. TPG is defined as the level of pressure gradient below which fluid cannot flow. When pressure gradient is larger than TPG and overcome the viscous forces, fluid starts to flow, which is always called as low velocity and non-Darcy flow. A mathematical single-phase flow model incorporating pseudo TPG is proposed to describe the flow behavior in low permeability reservoirs (Li et al., 2016). Fully implicit numerical simulation based on PEBI grid is developed to study the transient pressure response. Two field data are used to calibrate and validate the proposed model and the code. Based on one of field data, parametric studies are conducted to investigate the effect of minimum TPG, pseudo TPG and nonlinear exponent on the pressure transient response for a vertical well. We find that pseudo TPG can explain the unique and consistent characteristic of the pressure transient response in low permeability reservoirs. Our conclusions would be as follows. （1） Pseudo TPG can explain the unique and consistent characteristic of the pressure transient response in low permeability reservoirs, which is useful for petroleum engineers to interpret the field data. （2） The physics of upwarp of derivative curves is the lower flow speed due to pseudo TPG, which leads to large pressure change speed during med-late time. This also means that TPG is not the physics of upwarp of derivative curves for wells in low permeability reservoirs, which is not reported before. （3） Although the proposed corrected Darcy's law was validated by field data, the proposed model cannot describe all the flow behaviors in the low permeability reservoirs. Based on our experience of interpretation, the nonlinear function expression would be different for different low permeability reservoirs. The finding is useful for petroleum engineers to interpret the field data to obtain some basic parameters for low permeability reservoirs.

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Study on Waterflooding Performance in Low Permeability Reservoirs Using Stream Tube Method

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Based on the basic principle of streamtube method, the dynamic process of water flooding was simulated. According to the changes of the calculated dynamic indexes, the change rules of water drive performance were obtained. The two-dimensional two-phase displacement model was simplified to a number of one-dimensional streamtube models of triangle shape based on the characteristics of water flooding of five-spot pattern, so the triangle streamtube model of five-spot pattern was established. Then, the one-dimensional waterflood front equation was applied to the single triangular streamtube. With the relationship among the parameters in the streamtube, the position of waterflood front of different time was determined for each streamtube. Applying the equation of Darcy flow to the triangular streamtube, the resistance to flow was calculated when waterflood front before and after breakthrough. In this way, the dynamic indexes of water flooding could be calculated through the derivation in each streamtube. And then, superimposed onto the five-spot unit, a whole set of calculation equations for dynamic indexes was deduced, which are suitable for water flooding in the five-spot pattern. By means of this calculation method, dynamic indexes including oil production, water production, sweep efficiency, recovery percent of reserves, water-oil ratio, water saturation and resistance to flow varied with the change of the displacement process were calculated, therefore, the change rules of water drive performance were summarized. The method can well simulate the condition of underground flow, and it is also very flexible and efficient, so that it can provide the theoretical guidance for the development of oilfields with water flooding.

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A Thermo-Hydrodynamic-Mechanical Computational Model for Multiphase Flow in Fracturing Porous Media

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In this contribution, a fully coupled thermo-hydrodynamic-mechanical computational model for multiphase flow in a fracturing porous medium will be introduced. The geometry constitutes three domains: a matrix domain, a fracture domain, and a matrix-fracture domain. The matrix domain is a porous medium constituting solid and fluid phases, governed by poroelasticity, fracture mechanics, and Darcy's law. The crack domain is a cavity constituting solid and fluid phases, where the fluid flow is governed by the Navier-Stokes equations, and the crack boundaries are kinematically described by the solid phase. The matrix-fracture domain constitutes the fluid phase, governed by a leakage term derived based on Darcy's law. The domains are fully coupled in terms of the conservation of mass, momentum and energy. We adopt the representative elementary volume (REV) averaging theory for porous domain and the drift-flux model (DFM) for the fracture domain, together with the equations of state and constitutive relationships for the involved fluids and solid phases. We utilize a mixed discretization scheme to solve the governing equations. The standard Galerkin finite element method (SG) and the partition of unity finite element method (PUM) are tailored together to discretize both the continuous and discontinuous fields. The numerical examples shows that the proposed model is geometry- and effectively mesh-independent, making it computationally very efficient.

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Compositional Modeling of Two-Phase Flow in Porous Media Using VT-Flash

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We deal with the numerical modeling of compressible multicomponent two-phase flow in porous media with species transfer between the phases. The mathematical model is formulated by means of the extended Darcy's laws for all phases, components continuity equations, constitutive relations, and appropriate initial and boundary conditions. The splitting of components among the phases is described using a formulation of the local thermodynamic equilibrium which uses volume, temperature, and moles as specification variables in contrast to the traditional approaches using pressure, temperature, and composition. The problem is solved numerically using a combination of the mixed-hybrid finite element method for the total flux discretization and the finite volume method for the discretization of continuity equations. These methods ensure the local mass balance. The resulting system of nonlinear algebraic equations is solved by the Newton-Raphson iterative method. The numerical flux is discretized in a way that no phase identification nor determination of correspondence between the phases on adjacent elements is required in contrast to the traditional approaches. This is very important for the simulations of CO2 sequestration because, typically, CO2 is injected into a reservoir in the supercritical state at which the phase distinction is ambiguous. Moreover, our model performs well in situations where a phase appears or disappears and no switching of variables is needed. We describe the numerical model and show several 2D simulations, e.g. CO2 injection into water or oil saturated reservoirs.

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Numerical evaluation of multiphase flow processes and their effects on hydrocarbon production in hydraulically fractured reservoirs

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The combination of horizontal drilling and hydraulic fracturing – aka “fracking” – has enabled the creation of extensive fracture networks in extremely tight shale gas/oil reservoir rocks as a means to increase overall formation permeability. Production of shale gas/oil is then largely dependent on the immediate release of “trapped” hydrocarbon fluids intercepted by the hydraulically-induced fractures and the transient migration of hydrocarbon fluids from formation matrix rocks to nearby fractures. However, these processes may be further complicated by interphase mass transfer, extremely high fracture-matrix permeability contrast, and large capillary pressure occurring at the fracture-matrix interface, leading to multiphase flow behaviors that are different from those observed in conventional hydrocarbon reservoirs. Therefore developing a reliable model that is able to accurately simulate coupled multiphase flow and transport processes in hydraulically fractured shale or low-permeability rocks is of particular important for assessment of shale gas/oil production and evaluation of hydraulic fracture performance. There are two general modeling approaches that can be used to simulate multiphase flow in fractured porous media, namely, continuum and discrete fracture models. Most of current applied reservoir simulators, which typically employ “dual-continuum” conceptualizations for predicting hydrocarbon production of fractured shale reservoirs, are simpler to implement, but suffer from limitations in their fundamental conceptualization, and an inability to accurately represent fracture-matrix interactions especially when fracture-matrix permeability contrast is very large. For this reason in this study we have developed a discrete fracture model (DFM) in GEOS, which is a LLNL multi-physics computational code, to simulate multiphase flow and transfer in hydraulically fractured rocks. The DFM model is able to explicitly represent both individual fractures and their surrounding rock matrix, therefore providing a more precise representation of multiphase flow behaviors at the fracture-matrix interface which the continuum method is difficult to reproduce. We have further applied the developed DFM model to simulate multiphase (water, oil, and gas) flow and migration processes in fractured shale or low-permeability rocks under different hydraulic stimulation conditions. The stimulated discrete fracture networks used in the simulations are calculated by the hydro-fracture model (also implemented in GEOS). Numerical results show that both the viscous and capillary-driven fluid movements across the fracture-matrix interface tend to redistribute pumping and residual fluids within tight rock formations during hydraulic fracturing and hydrocarbon production steps, and greatly influence unconventional hydrocarbon production and fracturing fluid recovery. The DFM model developed in this study can not only help accurately describe effects of fracture-matrix interactions on multiphase flow processes in low-permeability formations, but also provide a useful interface to couple with the hydro-fracture model for accurate prediction and assessment of hydrocarbon production and hydraulic fracturing performance. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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Various alternative formulations of the flash equilibrium calculation

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Calculation of the equilibrium phase splitting(partitioning of the components between the phases) is one of the basic problems in chemical engineering with many applications in the energy industry, among others in compositional models, which are essential for simulations of processes related to enhanced oil recovery or CO2 sequestration. When a gas is injected into a porous and/or fractured reservoir, depending on the outer conditions, the mixture of gas and the reservoir fluid can remain in a single phase or can split into two (or more) phases. The task is to detect which of these two cases occurs (phase stability testing) and, in the multi-phase case, to determine the amount, densities, and chemical composition of the equilibrium phases (phase equilibrium calculation).

The standard way to formulate phase equilibrium problem in compositional simulators is to use minimization of the total Gibbs free energy of the system at constant pressure, temperature, and total numbers of moles of individual components. Alternatively, a system of equations for stationary points of the Gibbs free energy are formulated (isofugacity conditions) and these equations are solved using iterative methods. Many methods have been developed using this methodology.

No matter how standard this approach is, the formulation of the phase equilibrium using the variables pressure, temperature, and mole numbers (variables PTN) has several limitations that are mostly ignored in the literature. In this presentation, we will give an overview of several alternative formulations of the phase stability testing and flash equilibrium problems that we have investigated in recent years. These include formulation of phase equilibria in a system described by the total volume, temperature, and moles (variables VTN) and internal energy, volume, and mole numbers (variables UVN). We will present a unified formulation of the phase equilibrium problem that can include all three formulations mentioned above in a unified way. Therefore, a single solver can be developed to treat any of these three formulations. We will discuss properties of the individual formulations and show advantages of the alternative formulations for applications in compositional simulation.

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Characterization of fractured outcrop chalk using relaxation and relaxation exchange low-field NMR

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Fractured rocks are prominent for their high transport capacity and important in petroleum and ground water engineering, nuclear waste management, and civil and construction engineering. One specific carbonate rock, naturally fractured chalk, occurs as important oil reservoir (e.g. Austin Chalk, Ekofisk), while chalk stability is important in civil engineering and construction context. NMR relaxometry is a common technique to evaluate storage and transport properties of porous rock. Recent applications include 2D relaxometry (T1-T2) [1]. NMR relaxometry was applied to study pore structure and weakening of outcrop chalks [2] and pore characteristics of deformed chalk [3]. Carbonate systems often exhibit bi- and higher-modal porosity, altering relaxation time responses due to diffusional coupling or magnetization exchange between different pore systems [4-6].

In the limit of uniform properties of two populations such as chalk with large planar fractures or beads packs, such systems can be reasonably described using 1D approximations (similar to [4-6]). We re-evaluate the concept of additive magnetization of a two-type rock system. By respecting mass conservation through simulation we find that for high NMR contrast between rock types there is a statistically significant extra term describing spins originating mostly from the most mobile type of two rock-types. Experimentally, we consider T2-store-T2 relaxation exchange (REXSY) experiments [7] to characterize transport between different pore systems for water-saturated fractured chalk. The technique saw limited application due to relatively weak cross-peaks, which are susceptible to experimental artefacts caused by the ill-conditioned nature of the inverse Laplace transform [8]. In the T2-T2 exchange experiment the observed magnetization is the sum of five terms:

Mobs = M11 + M22 + M1b2 + M2b1 + M2b2,

where M11 and M22 are magnetization of spins relaxing predominantly in type 1 and type 2, M1b2 and M2b1 are mixed terms resulting from magnetisation exchange, and M2b2 is governed by the difference in diffusive transport (mostly spins of bulk water bounced back from the matrix surface). The presence of the latter term implies that T2-store-T2 maps of saturated fractured chalk exhibit five significant peaks, three of which are on the diagonal, plus cross-peaks of the faster components.

In this work we derive physical properties of a fractured system from observed NMR relaxation responses. By varying temperature and/or self-diffusion coefficient of fluids saturating chalk, we extract information about fractures using either a standard CPMG experiment or the T2-store-T2 technique. The main limitation for quantitative interpretation of results is signal noise and uncertainty associated with the 1D/2D inversion approach. We reduce this uncertainty by considering representative digitized representation of the chalk samples and also carrying out NMR T2 and T2-store-T2 experiments.

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Characterization of Interaction Between Oil/Brine/Rock under Different Ion Conditions by Low Field Solid-State NMR

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For the foreseeable future， water flooding will still remain the most economical and the most efficient way for oil field development and production. Apart from the conventional purpose of water flooding, which is to supplement energy into reservoirs and to support formation pressure, how to extend the function of water flooding is a key to enhance oil recovery while keeping the cost low enough. Currently, ions tuning water flooding(ITWF), with its function to adjust the ion strengths amongst ions of reservoir oil, clay minerals and injected fluid, rises as a hot-spot add-on that helps detach the crude oil from surfaces of clay minerals, hence enhances both micro and macro oil displacement efficiency. Quantitative investigation and evaluation of the microscopic mechanism of ITWF on oil/water/mineral is the key to the technical breakthrough. In this work, we suggested to use low field solid state NMR to evaluate the interaction between model oil compounds and inorganic rock interface under different ions tuning water. The fully refocused FID changed according to different water and ion used. Adding certain amount water weaken the interaction between model oil compounds and inorganic rock interface. However, ions strengthen the interaction between model oil compounds and inorganic rock interface, which played a negative role. The results could well guide our further application of ITWF.

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Coupled NMR-Minispec and MRI evaluations of the transport and clogging of non-colloidal particles in porous media.

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Understanding particle transport and deposition in porous media is key for a broad variety of processes, such as water purification, industrial filtration, or geosciences. This topic is here studied using flows of micro-scale particles through model bead packs (grains). Particles sizes are chosen to neglect colloidal interactions and physico-chemical adsorption, and focus on hydrodynamics: straining events (interception in narrow throats) or multiple-particle events (pore clogging by particle bridges).

Two types of NMR studies are performed to study the dynamics and statistics of such events. On the one hand, 1D profiles along the samples are made using a Minispec TD-NMR device. Despite its main use for high accuracy T1 and T2 measurements, it can also perform 1D imaging by adding a pulsed field Gradient Unit. On the other hand, MRI was used to map porosity and velocities in 2D layers of the samples.

Experiments have been carried out for particle/grain size ratios between 0.05 and 0.1, where straining events are known to predominate [4]. For ratios over 0.15 we get predominant caking on top of the porous media, as expected as the average particle size becomes bigger than the average pore size. In the study range, Minispec 1D profiles show progressive decrease in porosity and thus provide the average information on clogging. Clogged fractions are confirmed using the peaks variations of T2 distributions depending on the pores sizes, this is to say the amount of stopped particles in a given area. At the end, an exponential decrease of the clogging probability is verified over the height of the sample, which can be represented by a simple statistical model adapted from P. Coussot 2007 [5]. A striking result is the repeatability of the statistics for a wide range of particle size (at given particle/grain ratio), showing that the only events occurring are mechanical.

Additional studies of the structures created in the samples are conducted by MRI 2D mapping. Slice by slice analysis of MRI data allows to identify the clogging source and dynamics. By following the loss of signal in selected slices, we can quantify the increase of porosity heterogeneity and the development of preferential flow paths. A next step regarding MRI is to identify and study flow velocity images, for example provided by a classical phase-sensitive sequence (flow-encoded spin echo) as in [3,6].

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Effect of dry density and initial water content on the soil-water characteristics of compacted clayey sands：A NMR-based analysis

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Drying characteristic curves for two compacted clayey sands with different dry densities and initial water contents were measured, analyzed and compared. Based on the nuclear magnetic resonance (NMR) measurements, the effect of dry density， initial moisture content and soil composition on the drying characteristics of the compacted soils is investigated. The process was monitored by measuring capillary and adsorptive water contents, T2 distribution curves, T1-T2 spectrums and distributions of log (T1/T2) during drying process with NMR technique. All the results at various suctions were measured and used to characterize the moisture distributions in the soils, and the effect of the dry density， initial moisture content and soil composition on the drying process of the compacted soils were analyzed. The results show that the effect of dry density on the drying process is significant only at low matric suction, and for the soils with high matric suction, the effect of the initial moisture content and soil composition becomes important. Based on the analysis of the NMR measurements, it is also shown that in compacted clayey sands, the structure and content of micropores are mainly determined by the initial moisture content and soil composition, whereas those of macropores are controlled by the dry density. In general, soil composition has more significant influence on the internal structure and pore-size distribution of compacted soils than initial moisture content.

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Electro-kinetic penetration of lithium in concrete to mitigate ASR damages: an NMR study

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The deterioration of concrete by Alkali-Silica Reaction (ASR), commonly recognized as “the cancer for concrete”, is a well know phenomenon [1]. ASR is a chemical reaction that occurs in concrete between the alkalis, hydroxyl ions present in the pore solution and reactive silica, causing the production of ASR-gel. Due to its hygroscopic nature the gel imbibes water and swells to such an extent even to cause cracks in its surrounding concrete. The enhancement in its permeability due to cracking makes concrete more vulnerable to other damages such as the corrosion of reinforcing steel due to an increased ingress of chloride ions and sulphate attack etc. The effect of lithium compounds on the inhibition of ASR-gel expansion in concrete is known since several decades [2]. However, the relatively low porosity and permeability of concrete limits the possibility of Li penetration into sufficient depths under diffusion and/or hydraulic advection in a reasonable time scale. In order to penetrate Li more efficiently, electrochemical method is being used [3]. In this method mortar/concrete specimen is sandwiched between two compartments containing electrodes and electrolyte solutions. The anode compartment is filled with lithium-based electrolyte and cathode compartment is usually filled with saturated calcium hydroxide solution. Under the effect of an applied potential difference between electrodes, the Li ions in the anode compartment are repelled by the anode while attracted by the cathode to enhance their penetration speed into the specimen. Until now, the effect of applied electric field on the variation in Li ions concentration and its penetration speed in concrete is measured by using destructive methods. These methods are limited by their inability to measure variations in moisture and Li ions content in pore solution during electro-kinetic treatment. Moreover, in addition to a limitation in their spatial resolution (being general in the order of ~ 10 mm), some portion of the specimen is wasted during cutting, grinding and mixing processes while preparing samples for chemical analysis. Consequently, for this study non-destructive measurements are performed to study the effect of electric field on the migration of Li ions and variation in its concentration by using NMR. This study also includes the binding of Li ions on the pores surfaces and its influence on the migration of free Li ions.

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Estimating microstructural length scales in biopolymer hydrogels by PFG NMR nanoprobe diffusometry

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Biopolymer hydrogels constitute crosslinked, percolating polymer networks, giving rise to a porous and tortuous microstructure. Descriptors of that microstructure can be obtained from the reduced self-diffusion coefficients of embedded nonsticky nanoparticles with different size.1 If such nanoparticles are smaller than the structural features of the network, their mobility will be determined by “local” physical properties that may be different from the macroscopic properties of the gel. If the size of particles is smaller than, but on the order of, the distance between the polymer strands or fibers, the particles are still free to diffuse in the water phase, but their mobility will be impeded because of obstruction by the polymer strands. Particles larger than the structural features of the polymer network would be completely immobilized.1-4 For the largest part, however, diffusion of nanoparticles remains unrestricted but hindered. The pertinent question is what information can be obtained from this hindered diffusion. Physical models have been used to relate the reduction of nanoparticle self-diffusion coefficients to polymer concentration, polymer strand thickness, nanoparticle size and network mesh size.1,6 Many of these models try to capture the “obstruction effect”, i.e. the effect that the rigid and tortuous polymer network imposes an increased path length for particles moving between two points in the network. Such obstruction models predict long-term, average particle diffusion coefficients (assuming simple Brownian motion and a static network structure). Here we explore whether such models can adequately describe nanoparticles moving unrestricted through a polymer gel by using a set of equivalent spherical nanoparticles of different size. As a model biopolymer we have used κ-carrageenan, a naturally sourced linear polysaccharide that is widely used industrially as a gelling agent. Gelation of κ-carrageenan occurs upon cooling a warm aqueous solution. Gelation is very sensitive for binding of cations such as potassium, calcium, or sodium ions, to the polymer coils. The microstructure of κ-carrageenan gels can therefore essentially be controlled by the choice of cations, making it an elegant model system for microstructural studies. We have tested whether the self-diffusion behaviour of water, a low-molecular weight probe (ATEMP) and nm-scale dendritic nanoparticles can be modelled in a consistent manner. For the dendritic particles and ATEMP their (corrected) self-diffusion behaviour consistently predicted a polymer strand thickness of ~3.0 nm. The (corrected) self-diffusion behaviour of water could however not be fully explained by presence of proton exchange and network obstruction. This deviation might lie in the presence of regions with higher-viscosity (surface) water that are inaccessible for the larger particles. Such low diffusivity has been observed by Overhauser Dynamic Nuclear Polarization (ODNP)-enhanced NMR relaxometry by use of probes and nanoparticles functionalized with nitroxide-based paramagnetic TEMPO-spin labels. We discuss how we can reconcile the PFG NMR diffusivity with the ODNP-observed diffusivity and safely estimate the average mesh size of the network. Such information can aid in the validation of microscopic images of biopolymer networks.

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Experimental study of the drainage process in thin hydrophilic fibrous layer with LF NMR

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Among others, the NMR-MOUSE [3] has been used for the determination of the liquid distribution inside porous materials, such as detection of moisture in soil, concrete bridge decks, building materials and food [1,2]. In this study the NMR-MOUSE has been used for dynamic measurement of the drainage process through a thin porous layer. In a first experiment a slice with a thickness of 200 µm was excited inside the layer and the signal amplitude was acquire with a CPMG sequence. The CPMG echo train was Fourier transformed along the echo acquisition time to obtain signal intensity over time and position. T2 contrast was used to visualize the 1D liquid distribution with a time resolution of 50 ms and a spatial resolution of 20 µm over the thickness of the layer. Ongoing efforts aim at reducing the gradient strength of the magnetic field generated by single-sided sensors to increase the thickness of the excited sensitive volume without compromising the depth resolution of the sensor [3,4].

In order to address the inhomogeneous magnetic field in the depth direction a mathematical post processing approach has been established [5]. It uses the signal intensity of fully saturated filter paper as a mask function to normalize the signal amplitude of the filter paper during the fluid injection process with a constant flow rate of 80 µL/min.

In another experimental set up, the layer is drained by placing a layer of same material underneath the top layer where capillary forces are driving the drainage process. The main objective in this measurement is to monitor dynamic drainage process of a thin nonwoven porous material. To this end, the fully saturated layer was placed on top of a dry layer, and the signal amplitude was acquired in the sensitive slice with employing the CPMG sequence.

This study demonstrates a promising method to non-invasively explore the dynamics of liquid ingress into a thin fibrous porous material. The features of the low-field unilateral NMR measuring device excellently match the geometry of the system of interest, thus allowing a suitable choice of spatial and temporal resolution. This match of geometries also shows that frequency encoding of the depth direction can be used, rather than physically moving the instrument relative to the sample as is usually done.

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Imaging of 23Na accumulation in the soil-root region due to root water uptake

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Root water uptake may lead to salt accumulation at the root-soil interface, resulting in rhizophere salt concentrations much higher than in the bulk soil. This salt accumulation is caused by soluble salt transport towards the roots by mass flow through the soil, followed by preferential absorption of specific nutrients by active uptake, thereby excluding most other salts at the root-soil interface or in the root apoplast. The salinity build-up can lead to large osmotic pressure gradients across the roots, thus effectively reducing root water uptake and crop production. The increased salinity also leads to a deterioration of soil quality and, eventually, to the loss of productive crop land. Therefore, an understanding and a description of the processes taking place are required, in terms of parametrizing soil physical models. To start with, reliable measurements of the salt accumulation in the soil and the roots are needed. Therefore, we present 23Na-MRI for the visualization of NaCl distribution in the soil-root region, complementary with 1H-MRI for high resolution imaging of the root system and the water content development for providing synergistic information about the underlying water flow and solute transport processes. While common in medical research, 23Na-MRI is not very well developed for unsaturated porous media such as soils. The 23Na NMR signal is much weaker than the most common 1H signal due to the lower gyromagnetic ratio and the much lower abundance. This results in a lower resolution and requires longer measuring times, which is facilitated by the relatively short T1 in the range of about 50 ms. In this pilot study, we used a fast spin echo method with tE = 5ms, 16 echoes and a matrix size of 32 x 32 x 32, yielding an FOV of 32 x 32 x 64 mm. For the calibration phantom, we showed that the MRI voxel intensity was proportional to the 23Na concentration down to a concentration of 0.05 mol/L (Fig. 1a). This allowed us to apply this procedure to the accumulation of 23Na in the root systems of tomatoes, which were irrigated in three-day intervals with a 0.06-M NaCl solution. After 10 days, we found considerable salt accumulation in the root region, which could be used in the second step to alculate profiles. New perspectives could be obtained by co-registrating these data with the 1H2O-MRI of the root system architecture and soil water content.

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MRI measurement and numerical simulation of coupled fluid flow and heat transfer in phase change material (PCM) porous media

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Non-isothermal packed bed systems are important in a range of applications including catalytic reactors and emerging thermal energy storage (TES) technologies. Within TES, phase change materials (PCM's) are being applied in a broad range of systems from molten salts for high temperature thermal energy storage to particle encapsulated waxes in building materials. In this study, packed beds of core shell wax particles serve as a template system to study the behavior of the melting waxes and show the performance of the packing arrangement during non-isothermal flow situations. The magnetic resonance imaging (MRI) method relies on the molten wax generating signal while the solid wax does not, providing the spatial temperature distribution once a phase transition has occurred. This work studies this effect in several arrangements including microencapsulated (~15 um) and macroencapsulated (~5 mm) beads with heating from either an outer annulus or through bed flow. Numerical simulations of the fluid flow and transient thermal behavior during phase change are included in each arrangement. MRI measurements of spatial fluid velocity using 19F NMR and temperature distribution in the particle phase using 1H NMR, of the bed demonstrate the pore scale coupling of mass and energy transport by individually resolving the fluid and particle phase by NMR active nuclei. MRI measurements using standard spin warp imaging provide high spatial resolution ~50um velocity and temperature data averaged over ~10min while rapid imaging methods provide coarse grained ~500um spatial resolution data of transient thermal variations on time scales of ~1s. A range of Reynolds number and mass and heat transfer Peclet numbers are considered in natural convection and pressure driven packed bed flows.

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NMR relaxation in partially saturated pores: applications to cement paste and carbon xerogels

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Nuclear magnetic resonance (NMR) relaxometry techniques are widely used for the characterization of porous materials. They exploit the proportionality between the relaxation rate and the surface to volume ratio of the investigated pores. The proportionality constant, also called relaxivity, is determined by the adsorption properties of molecules on the pore surface [1], the magnetic impurity content of the solid matrix [2,3] and the magnitude of the external magnetic field [1-3]. Consequently, the relaxation experiments provide us access to the pore size distribution and the wettability of the confined fluids. Most NMR relaxation studies of molecules confined inside porous media refer to saturated conditions. In fact, saturated conditions are a priori assumed in many applications (cements, soils, xerogels), even if in reality we have to deal with partially saturated pores. That is why, in the present study the relaxation of molecules under partially saturating conditions was considered as a function of filling degree and a new model for the effective relaxation rate was introduced [4,5]. In the frame of the new model the relaxation rate is also a function of the filing degree of the pores. As an application for the new model the relaxation of water and cyclohexane molecules partially saturating a white cement paste and a carbon xerogel was considered. The two porous materials with nanometer sized pores were selected due to their different surface properties. The two filling liquids were selected as representatives of polar (water) and nonpolar (cyclohexane) molecules which should experience different interactions with a surface containing OH groups of the cement paste [2]. Stronger interaction was observed in the case of water filled porous cement as compared with the cyclohexane filled case. This property was exploited to clearly identify the different categories of pores in cement paste with pore sizes ranging from nanometers to micrometers. It was also observed a different drying process of the three types of pores and a different molecular distribution inside these pores. In the case of xerogel sample the cyclohexane revealed stronger interaction with the surface. This behavior was attributed to the interactions between the sp3 hybridized carbon atoms of cyclohexane and the sp2 hybridized carbon atoms in the structure of the synthesized xerogel [6]. Information about liquid distribution under partially saturated conditions could be also extracted.

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NMR relaxometry investigations of molecular interaction with clean and paramagnetic surfaces

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NMR relaxation, in particular its field-dependent variety NMRD, has been proven to be a strong indicator of anomalous molecular dynamics at surfaces. It is known for decades that in pores of untreated glass, the polar surface leads to a residual average orientation of polar adsorbate molecules (water, alcohols) which, in turn, give rise to extremely long correlation times due to a process called bulk-mediated surface diffusion [1]. A similar trend has been observed for unpolar hydrocarbons in inorganic mesoporous materials, where a surface coverage with coke leads to a dramatic increase of relaxation dispersion in organic liquids [2], while leaving macroscopic diffusion properties largely unaffected. It is not yet clear whether this is due to a much stronger interaction of fluid molecules with the surface, or to the existence of additional relaxation sinks such as stable radicals. More recently, it was demonstrated that radicals indeed play an important role in relaxation dispersion of fluids with asphaltene aggregates either in crude oil or diluted in solvents: asphaltenes naturally contain stable radicals and paramagnetic ions. In addition, relaxation is much more pronounced for aromatic than for aliphatic molecules, suggesting pi-pi stacking leading to extended lifetimes of the molecules close to the surface [3,4]. While relaxation can be modelled partly by taking the tumbling of asphaltene aggregates into account, the same trends were observed in the immobile environment of bitumen, which has a composition similar to asphaltene. In this study, the interaction of solvent molecules with the solid hydrocarbon surface of porous catalyst carriers and porous asphaltene aggregates is compared and discussed in terms of a refined model of molecular dynamics in dependence of aromaticity and polarity.

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Non-destructive measurements of chloride migration in concrete by NMR

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The chloride-induced corrosion is widely recognized as one of the main degradation mechanisms in civil structures based on reinforced concrete. The corrosion starts as soon as the chloride comes in contact with reinforcement steel bars [1]. In general the chloride enters a concrete by advection with moisture or diffusion within the moisture present in concrete. Gaining insight into these transport phenomena can not only improve the assessment of durability aspects of existing structures, but might lead to improved design for new reinforced concrete structures that are to be used in aggressive environments. In order to investigate the transport of Cl ions in concrete several laboratory testing methods have been developed, however, due to its short duration (varying from 6-96 h), an accelerated test method [2] commonly known as the Rapid Chloride Migration (RCM) test is widely preferred. In RCM test a concrete specimen initially saturated with calcium hydroxide solution is sandwiched between two compartments containing electrodes (anode and cathode) and electrolyte solutions. The cathode compartment is filled with NaCl solution (~ 2 mol/dm3), while the anode compartment is filled with NaOH solution (0.3 mol/dm3). Under the effect of an applied potential difference between electrodes the chloride ions migrate from cathode to anode within the concrete specimen. After the completion of test the specimen is split and the penetration of chloride in concrete is measure by spraying a colorimetric indicator i.e. AgNO3 for the determination of chloride content. The rapid diffusion coefficient DRCM based primarily on the penetration depth of chloride as measured by color indicator is further used for modeling the chloride transport in concrete. Since several factors e.g. alkalinity of concrete, different parts of specimen exposed to different amounts and the variation in concentration of AgNO3 might influence the color change boundary and thus the DRCM. In addition to that this measurement method does not provide any information about the distribution of moisture and transport of Na ions and their effect on migration of chloride in concrete. To overcome these shortcomings transport of chloride ions during RCM tests is being measured non-destructively using NMR. Our NMR setup provides a unique opportunity to measure moisture, sodium and chloride ions quasi-simultaneously in concrete [3]. The data obtained will provide more realistic values of diffusion coefficient of chloride in concrete. The binding effect of chloride ions with concrete and its interaction with sodium ions on the transport of free chloride ions will also be a part of this study.

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Nuclear Magnetic Resonance for fluids in porous media: Applications for Cultural Heritage, Environmental Sustainability and Human Healthcare

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Nuclear Magnetic Resonance (NMR) offers different techniques that have become increasingly important tools for investigating pore space structure as well as pore surfaces and fluid properties in a wide class of heterogeneous high surface-to-volume ratio systems, of natural or synthetic origin, of organic or inorganic nature. Porous rocks [1], cements [2], gels as well as biological systems as bone, cells, corals [3] and food are in the mainstream of materials studied. Structure, fluid-flow properties, water absorption, water diffusion and exchange among compartments are typical phenomena examined. This work depicts NMR applications to different fields in which the same techniques, data-acquisition methods and data-analysis algorithms can be applied to get unique information from systems characterized by a wide range of scale lengths, which in some cases can span from a few nanometers to the macroscale level. These techniques were applied to both solid porous media of interest to Cultural Heritage and biological systems that, for many aspects, can be considered as porous media. The results of measurements in highly homogeneous magnetic fields and in the presence of the magnetic field gradient of single-sided devices are presented. Most relevant NMR techniques applied in this study are Relaxometry (in 1 and 2 dimensions) and Imaging (MRI) of 1H nuclei of liquid water confined inside the pore space of the porous materials. In particular, MRI can be applied to visualize in a non-destructive manner internal sections of porous media saturated with water [1], with the possibility of 3D reconstructions of the structure of the pore space occupied by water. While imaging allows one to get information at the sample-scale, relaxation data give information at the pore-scale. Relaxometry and MRI can be combined in Relaxation-Imaging, which allows the spatially-resolved study of NMR parameters connected with the pore space. In this work, we show applications of NMR techniques to Cultural Heritage, Environmental Sustainability and Human HealthCare.

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Pore Structure Characterization of Shales Using NMR Cryoporometry

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Considering that most matrix pore sizes of shale rock are at scales of a few nanometers to microns, charactering Nano-pore and understanding the pore structure are therefore significant and imperative for shale gas production. However, to accurately characterize the pore structure of shale remains a challenging task in geoscience community due to the complexity and heterogeneity of the shale pore structure. There are various techniques for characterization of pore structure properties, such as Scanning Electron Microscope (SEM), Mercury Intrusion Porosimetry (MIP) and Nitrogen Adsorption Method (NAM) and X-ray Computerized Tomography (XCT), but each of them has a limited measuring range and could not cover the entire nanometer-range. This work reported nano-pore characterization of shale rock in Sichuan, China using nuclear magnetic resonance cryoporometry (NMRC), a novel and emerging technique which can probe pore size distributions from nano- to micro- scales. First, the method was validated using two materials with pre-known pore structures, a molecular sieve SBA-15 with a pore diameter of 8 nm and a controlled pore glass with a pore diameter of 24 nm. The NMRC results of two martials show a good accuracy for quantifying pore size distribution. Both bulk matrix specimens and pulverized shale samples were tested using NMRC, and two liquids, water and cyclohexane, were used to saturate the samples for NMRC experiments. MIP, NAM as well as NanoCT were also employed to validate the NMRC results. The results show that MIP was comparable to NMRC with bulk sample and NAM was similar to NMRC with pulverized sample. The porosity for bulk and pulverized sample is 3.2% and 5.7% respectively, showing that a lot of pores were connected during pulverizing process. The results for samples saturated with water and cyclohexane are similar, which demonstrates that water-rock interaction was not active during experiment due to the low temperature. However, cyclohexane has a greater Gibbs-Thomoson coefficient than water, meaning that NMRC with cyclohexane has a better resolution, but water molecular is smaller, making it easier to imbibe to nano-pores, which are also showed in the results. Combing with NanoCT and FIB-SEM images, the applicability of pore structure characterization of NMRC was also studied. To summarize, NMRC can be a promising and powerful tool for pore characterization for gas shale when combined with other techniques including NMR relaxometry, spectroscopy, diffusion, and imaging.

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Porosity and permeability of coals at elevated temperatures investigated by nuclear magnetic resonance (NMR)

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For the past decades nuclear magnetic resonance (NMR) technology has gained acceptance as petrophysical tool for evaluating petroleum reservoir quality. Comprehensive reservoir evaluation requires determination of irreducible fluids, movable fluids and permeability. Although the NMR properties of fluid-saturated coals have been studied for decades, the temperature dependence of these properties (pore size distribution, pore structures, porosity and permeability) has never been systematically investigated. Thus, NMR experiments after elevated temperatures (from 25℃ to 375℃) were designed to study the variation of petrophysical properties of three rank Chinese coals. Results show that NMR transverse relaxation (T2) distributions strongly relate to the coal pore structure and coal rank. Based on T2 cutoff time method, five models for evaluating the permeability of coals were used. The results show that the Schlumberger Doll Research (SDR) model its improved models give much better estimation than the other models because these two models generally can represent the matrix permeability of coal based on the comparisons between the result from measured gas permeability and the results from NMR permeability models. Further calculations indicate that all of three different rank coals have an increasing trend with elevated temperatures, but differential increments exist among the coals. The medium rank coal has a maximum increment (9.44%), which can improve more than 200% of the original porosity (4.02%). While the permeability has no identical relationship for these three rank coals after elevated temperatures due to the strong heterogeneity of pores structure in coal reservoirs. For high rank coal, firstly the permeability goes up (from 0.52 mD to 0.61 mD) at low temperature stage (<75 ℃) and then drops down (from 0.61 mD to 0.5 mD) at high temperature stage (>225 ℃), which looks like an arc. This result demonstrates that the mcirofractures possibly extend their width during the heating process at low temperature stages, and then more micropores generated in coal matrix, in turn, which caused the mcirofractures width decrease because of the volume swelling in coal matrix. Therefore, they may have significant implications for the effects of heat from geothermal dynamics and magma intrusion on coalbed methane concentration and migration.

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Quantitative use of Magnetic Resonance Imaging data: application to tracer experiments in soils

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Quantitative estimation of flow and transport parameters is particularly important in soil physics, notably to predict water and nutrient availability for plants, aquifer recharge or contaminant transport. One common way to study this problematic is to resort to tracer tests. Generally, data provided by such tests are breakthrough curves presenting the arrival of tracer at the outlet and are used to assess the hydraulic properties of the material by parameters estimation. In this classical approach, these properties are representative of the sample as a whole, but do not allow to distinguish easily several materials. Moreover, the presence of heterogeneous soil structures (such as macropores) may induce different flow velocities inside a same material making the interpretation of data more difficult.

To solve this problem, one may resort to spatially resolved scanning methods. X-ray microtomography and Magnetic Resonance Imaging (MRI) are probably the methods that offer the best performance in terms of resolution, allowing, for example, the mapping of fine soil structures and the distinction between different materials. Although more sensitive to noise than X-ray CT, MRI allows nevertheless: 1) the optimization of the image contrast, notably by using convenient tracers and acquisition parameters (Cuny et al. 2015) and 2) the use of tracers that behave like pure water in soil. In this contribution, we evaluate the benefits of using MRI to infer soil hydraulic properties by performing tracer tests.

We first built a phantom sample with two different materials (sand and silt) set in a column according to a complex geometry. The sample was then put into a 4.7 T Bruker scanner and irrigated with tap water before the injection of the tracer: Gd-DTPA2-, a contrast agent known to enhance T1 and T2 relaxations. The process of tracer infiltration was monitored with MRI. In order to probe the signal before its very fast relaxation, we used an Ultrashort Time-to-Echo (UTE) pulse sequence with very short repetition time so that the whole sample was imaged with a high resolution (500 to 700 μm) in a relatively short time frame. After the experiment, 3-D UTE intensities were converted to tracer concentrations using the methodology proposed in Gharagouzloo et al. (2015) and initially developed for medical applications. A flow and transport model was built in HydroGeoSphere (Therrien et al. 2010) using semi-automated 3-D segmentation of materials based on MRI data. Tracer breakthrough curves at different locations in the sample were extracted from MRI datasets and fed into the parameter estimation software PEST (Doherty et al. 1994). Estimated hydraulic properties of the different materials based on MRI data proved to be consistent with values provided by material manufacturers.

The same experience was repeated with “real” soil samples collected on the field (Selhausen - Germany) providing also interesting results, though the presence of magnetic impurities still limits the quantitative application of the technique for such complex samples. The latter result puts in evidence the need to develop new or adapt existing acquisition sequences that should be less sensitive to magnetic field inhomogeneity.

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Refractory spalling of castables during first-drying: an NMR study

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Refractory spalling of castables during first-drying: an NMR study

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Monolithic refractories are a class of materials that exhibit optimum physical, chemical, and thermal properties at elevated temperatures. As specimens chosen for high-temperature use (over 1000 °C) in metallurgical applications, refractories must be designed to sustain high strength in the most extreme physical, thermal and chemical environments[1]. At this moment though, the more standardized type of refractory that has come to dominate the metals industry is a family of aluminous compounds, called castables. These particular refractories are used in the linings of hot ladles where steel is forged and extracted for mass production. However, under aggressive heating schedules (~10-20 ^{0}C/min), free and chemically bound moisture will be converted into liquid vapour over time. Consequently, this phase change generates high steam pressures within the pores that may approach the tensile strength of the material, resulting in dangerous explosive spalling and service failure[2]. In order to ensure that the free and chemically bound water components are removed from the porous matrix, the refractory elements must be slowly pre-dried for 30 hours until 400 °C.

In this study, two calcium alumina (CA) based conventional castables (CC) are prepared and cured for 24-48 hours and 48-72 hours, then subjected to one-sided heating for a duration of 1-2 hours within the temperature regime of first-drying (100-300 °C). The quantitative moisture loss and corresponding temperature profiles are simultaneously and non-destructively measured for continuous periods of time. The measurements are performed with a specialised high-temperature 1.5 T Nuclear Magnetic Resonance (NMR) setup.

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Simulation of tracer transport and root water uptake by white lupine (Lupinus albus L.) with R-SWMinisymposium

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Understanding and modelling root water uptake distribution is crucial to better manage water in agriculture. However, direct measure of soil water fluxes is still challenging. In this study, we combine a tracer experiment and modelling to estimate the 3-D distribution of root water uptake in a soil column.

The monitoring of the movement of an inert tracer (Gadolinium (Gd)) in a sandy column with a plant was performed with Magnetic Resonance Imaging (MRI) by Haber Pohlmeier et al. (unpublished). The experiment took place in a 10 cm high cylindrical column with a 5 cm inner diameter filled with natural sand in which a white lupine plant has been grown. The experiment and imaging started 18 days after seed germination. Irrigation was applied during 6 days and the column was imaged once per day during 7 days. The R-SWMinisymposium model (Javaux et al. 2008) was used to simulate this experiment. The boundary conditions were expressed in fluxes at the top of the soil column (evapotranspiration rate and irrigation rate with a 1 mmol/L Gadolinium solution) and in pressure head at the bottom (- 11 cm). The root system architecture (RSA) was manually reconstructed from the MRI data and then adapted by using Matlab routines for setting root origination time and root order before being used as input file in R-SWMinisymposium .

First, a virtual experiment was performed to assess the information on root water uptake which was available under this experimental set up. It was demonstrated that, when irrigation ceases, Gd concentration change was proportional to cumulative uptake. In addition, tracer distributions obtained by MRI and simulation were compared for a vertical slice located in the middle of the soil column. Tracer spatial distributions during leaching time (day 1 to 6) do not match, which could be explained by the fact that soil heterogeneity, that influences water distribution, is not included in the model. However, spatial distributions at day 7, which depend mostly on root water uptake patterns, match well. Therefor, tracer concentration distributions have been quantitatively analysed for day 7. It has been found that the concentration diminishes, both in MRI experiment and in the simulated results, when the distance to the nearest root segment increases.

To conclude, it seems that the simulated results match well with the experimental ones when root water uptake pattern has a bigger influence on water movement than soil heterogeneity (i.e. when irrigation is stopped). The results always have to be cautiously interpreted. Indeed, MRI technique has limitations in terms of precision and simulated results come from a model with simplifying hypotheses.

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Two-phase flow through sandstones using T2-resolved low-field NMR flow propagator measurements and simulations

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Understanding two-phase flow is critical in reservoir engineering for forecasting production rates and enhancing ultimate hydrocarbon recovery. NMR is an established well logging and laboratory technique used to measure a variety of petrophysical properties of rocks. Flow propagators are considered a useful tool to describe multiphase transport in rocks [1] due to their sensitivity to fluid movement, rock wettability state and its change. NMR propagators were derived experimentally and numerically to study two phase flow in clean sandstones (Fontainebleau) using high field 85 MHz system, Tessier & Packer (1998) [2], Packer et al. (1998) [3]. Grain packs and beads packs were studied using 20 MHz systems, Guillon et al. (2013) [4], Chevalier et al. (2015) [5]. Here we consider an application of two-phase flow propagators using low-field 2 MHz NMR. We simulated T2-resolved two-phase flow propagators using a combination of lattice Boltzmann methods, Arns et al. (2004) [6] and random walk methods, Schwartz and Banavar (1989) [7]. The first technique is used to obtain the velocity field, and the second to reproduce molecular diffusion. Simulations were performed on high resolution segmented tomograms of uniform bead packs, and Bentheimer and Castlegate sandstones. For the case of Bentheimer sandstone we imaged fluids distribution of oil and water set by steady-state flow at various fractional rate ratios, Zou et al. (2016) [8]. We also simulated oil-water distributions using morphological capillary pressure (drainage) transforms (CDT) following Arns et al. (2005) [9]. Assuming reasonable match between these two approaches, we applied the latter to beads pack and Castlegate sandstone digitized representations. This enables us to perform two-phase propagator simulations on three different morphologies. The relaxation dimension is added to relate local pore-scale dimension and fluid type and saturation to conductance of each fluid given by two-phase longitudinal propagator. We measure flow propagators of each of two phases separately in each of three samples. Isolation of oil response is achieved by using deuterated water to exclude contribution of a signal from the aqueous phase. We investigate the influence of surface relaxivity on low-field NMR two-phase flow propagators in sandstone rock at different saturations and fractional flow rates. This provides another insight into the concept of a local propagator, which refers to a propagator measured over a short encoding interval, which makes it free from mixing, Zheng et al. (2016) [10]. We validated average longitudinal propagators accessible via NMR simulations on high resolution micro-CT images by experiment for a range of dispersion times and Peclet numbers. We successfully applied numerically simulated two-phase T2-resolved flow propagator for enhanced interpretation of experiment to decompose acquired signal into the relative fraction of stagnant and mobile oil and water in respect to relaxation environment. We found that the addition of the relaxation dimension to flow propagator has potential for quantifying reactive processes and wetting phenomena in porous systems.

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Water content in natural soil by low-field NMR

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Soil moisture maintenance is significant for farmland irrigation and plant nutrient management to manage water flow and solute fluxes. Soil moisture is usually measured via the water pressure in soil system. There are several direct and indirect methods to characterize the water content in soil. Nuclear magnetic resonance (NMR) and remote sensing are two new emerging technologies owe great potential to characterize soil moisture. However, it is essential for soil-moisture maps acquired by remote sensing instruments from aircraft or satellites to be calibrated and validated by locally measured ground soil moisture data. NMR is one of the most powerful characterization methods with the ability to determine the absolute soil water content. The outstanding advantage for NMR is that it is non-invasive and does not require the investigated sample to be opaque or viscous. Therefore, NMR is an appropriate tool to characterize the fluid dynamic properties in soil science today. For decades, applications of NMR to soil science were restricted by the lack of portable and affordable instruments. Due to the fact that the instrument rests inside the object, this type of NMR is also named inside-out NMR [1]. At present, many small and portable NMR instruments with permanent magnets in open and closed are available for fluid dynamics studies of porous media. The small-scale NMR sensors with open magnet geometry contribute enable on-site field measurement and investigations of large objects with peculiar geometries. Two popular unilateral NMR instruments with open magnets are inside-out well-logging tools [2, 3] and the NMR-MOUSE® (NMR-Mobile Universal Surface Explorer) [4], respectively. Both devices can be taken outside for non-destructive studies of large objects such as studies of water in soil. In this work, the relationship between the acquired NMR signal and the true ground soil water content was studied and first results quantifying the water content for the Selhausen (TR 32 field site) bare field soil with an improved slim-line logging tool (SLL tool) and the NMR-MOUSE® in field and laboratory studies are presented. The work is part of the interdisciplinary project TR 32 funded by the DFG. The true soil water content from prepared samples was obtained by thermogravimetric method. The relationship between NMR determined and calculated soil water content and true volumetric soil water content (here 'predicted') is presented in Figure. 1. It shows that the NMR derived soil water content is the volumetric water content and that it scales linearly with the true volumetric soil water content. A linear regression of the NMR data generated R2 values of 0.98 and 0.96 for the NMR-MOUSE® and the SLL tool, respectively. Furthermore, a detailed calibration procedure between NMR measured water content and true ground water content was elaborated in this work. The results provide a model for calibration of the acquired results from the field site. This work indicates that the NMR-MOUSE® and the SLL tool are well suited for the measuring the volumetric soil water content in the field. These two mobile low-field NMR devices complement each other very well in field studies, as the NMR-MOUSE® could explore the field soil surface layer (2 mm-2.5 cm) and the SLL tool can be inserted into a hole in the soil several meters deep for monitoring soil water information.

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Wick action in porous materials as studies by NMR

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Salts crystallization is one of the main degradation mechanisms of historical heritage objects, such as masonry. Moisture penetration can drag dissolved salt along with it into a porous material. The salt can accumulate and crystallizes in the pores and can as a result produce cracks due to crystallization pressure. To get a better insight into salt transport mechanism we picked up a special situation when a porous material is in contact with salt solution on side and the same time is exposed to drying conditions on the opposite side. This situation is often encountered in cultural heritage where for example a masonry wall is in contact with groundwater, or open water as is often seen in the case of the historic city of Venice. This continuous transport of a salt solution, combined with drying, is referred to as wick action. During wick action salt ions will penetrate by two main mechanisms, advection and diffusion. The net ion flux will be a competition of these two processes. Due to the continues flow of salt ions towards the drying face there will be a continuous accumulation and as soon as the maximum solubility limit has been reached, there will be crystallization, either inside the materials (subflorescence) or outside (efflorescence). In this study we have focused on equilibrium wick action, when the conditions of exposed faces to the solution and air are stationery and porous medium stays water saturated throughout the process, i.e., without forming a drying front inside of the material. Hence we do not take into account the changing of the boundary conditions as would be seen in situ, i.e., due to changing weather conditions. In this study we have used Nuclear Magnetic Resonance (NMR) to measure both moisture and ions nondestructively and quasi-simultaneously during wick action experiments. These experimental results have been compared to a numerical model for advection-diffusion equation

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Analysis of monotonic and cyclic undrained behaviour of laterally loaded short pile foundation in dense sand with geo-centrifuge experiments

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Short pile foundations have been vastly used within the offshore and construction industry. The common methodology to analyse the interaction between soil and laterally load pile relies on the p-y curves concept. The method has a shortcoming since it is based on series of empirical data of slender pile field testing (LeBlanc, et al., 2010). Although it has been widely used to predict the ultimate pile lateral capacity prediction, a demand of more applicable method occurs. More and more practices require not only the safe range of ultimate capacity, but also more explanation of soil-pile behaviour during cyclic or static loading over time.

A study was conducted on the application of short pile as temporary anchorage of dredging vessel called Cutter Suction Dredge (CSD). The short pile element is called spud pole. The loading was characterised by the vessel movement due to the cutting process and the hydrodynamic actions of the waves. An experimental programme was developed to inspect the behaviour of spud pole as short a pile foundation under undrained lateral load. The lateral loads were distinguished into a set of cyclic lateral load that represents waves action, and a monotonic lateral load representing the large cutting force from the cutter head of the dredge. These lateral loads are applied perpendicular to each other. Several previous researches on multi directional laterally loaded piles were taken into account for developing hypothesis on this system (Su, et al. (2014) and Mayoral, et al., (2016b))

The experiment employed physical modelling work with geo-centrifuge. The tests were performed on two type of sand with different averaged grain sizes, mineralogy, and hydraulic conductivity. The samples were constructed to reach dense packaging with more than 70% relative density and at high degree of saturation rate of more than 90 %. A fibre based viscous fluid was used as pore fluid to satisfy the conflicting scaling of dynamic time and diffusion time. The sensors were design to capture the load and displacement at pile head, and pore pressure changes at the interface of the soil and pile.

The experiment proved that a laterally loaded short pile behaves differently than what is predicted with the available (conventional) p-y method. Contrast to the plastic softening behaviour, the short soil-pile interaction tends to have hardening pattern along with increased displacement. This is supporting previous findings from Le Blanc, et. al. (2010) and Zhu, et. al. (2015).

The explanation comes partially from the hydro-mechanical process of the undrained loading on saturated dense sand. The densely packed sand experienced grain re-arrangement during shearing, whether it was monotonically or cyclically sheared. The grain re-arrangement was followed by pore fluid response that oppose the tendency of sand package to contract, resulting in higher effective stress state. Additionally, the mechanism of laterally loaded short pile generated active and passive soil pressure. When these two pressure distribution are properly assessed and combined, they will

result in higher lateral response compared to what is predicted with conventional p-y curves that based its theory on flexural/long piles.

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Backward erosion piping: grain pore water flow interaction on different scales

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backward erosion piping, scaling, physical model tests, groundwater flow, grain transport.

Backward erosion piping is difficult to study systematically in the field, because of a large number of relevant but varying parameters as: grain size, permeability, thickness of soil layers, density, water levels. Model tests are therefore used to study the complex sand-water-grain mechanism that leads to backward erosion piping. This behaviour can only partly be studied with numerical models and also when numerical models can be used, validation of these by physical model tests is required.

However, the interpretation of scale model tests for backward erosion piping is hampered by scale effects. These scale effects are caused by the test requirement that the same grains have to be used in the model as in prototype to get meaningful results. As a consequence, model tests are performed at different scales and model tests are used in combination with analytical and numerical models to come to useful results. The use of model tests has increased our understanding of the processes and the influence of various boundary conditions is now much clearer. Future tests will be used for a better understanding of the influence of heterogeneity on back ward erosion piping and to study possible mitigating measures.

The presentation will show how scale effects occur and why these cannot be avoided in scale model tests and how these tests nevertheless are used in a combination with calculations to develop our understanding in the erosion processes. Furthermore, it will be shown how the backward erosion process develops at a grain scale level.

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Centrifuge modelling of root-induced soil suction and root geometry on slope stability

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Soil bioengineering using vegetation has been recognised as an environmentally friendly solution for shallow slope stabilisation. Existing studies have focused on the use of plant roots with different geometries to mechanically stabilise soil slopes, but there are little data available on the contribution of transpiration-induced suction to slope stability. Any additional induced suction would not only decrease soil hydraulic conductivity (hence rainfall infiltration) but also increase soil shear strength. These plant hydrological effects are often ignored in slope stability calculations.

This presentation will share a new physical modelling technique to simulate plant-induced suction and its application to study the plant effects on slope stability in a geotechnical centrifuge in the Hong Kong University of Science and Technology. The first part of the presentation will introduce a newly-developed artificial root system (Fig. 1; Ng et al., 2014) that is able to capture both the mechanical root reinforcement and hydrological effects of plant-induced suction. The artificial root is made of a high air-entry value porous filter, cellulose acetate, which has scaled mechanical properties, including tensile strength, elastic modulus and axial rigidity, similar to living roots. The performance of the system will be reported by comparing with laboratory and field data of plant-induced suction. The second part of the presentation will present a number of centrifuge test data that aims to explore the combined effects of transpiration-induced suction and mechanical root reinforcement to the slope stability subjected to rainfall (Fig. 2). Influences of different root geometries (i.e., tap-, heart- and plate-shaped; Ng et al. 2015) and slope gradient (45 versus 60 o; Leung et al., 2016) on the stability and failure mechanisms will be discussed. Relative contribution of mechanical root reinforcement and hydrological effects of plant-induced suction to slope stability will be highlighted.

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EXPERIMENTAL EVALUATION OF REYNOLDS NUMBERS AND LIMITS OF DARCY'S FLOW REGIME UNDER VARIATION OF GRAVITATIONAL FORCES AND CHARACTERISTICS OF POROUS MEDIA

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Among the useful applications of geotechnical centrifuge modelling techniques, increments of self-weight have been widely used to study the flow phenomena through soils. The possibility of inducing high values of hydraulic gradients due to the increment of the centrifuge gravitational force in a model has allowed the investigation of flow through fine-grained soil for which very low permeability values are experienced (Nimmo and Mello, 1991; Singh and Gupta, 2000). However, as indicated by Goodings (1994), the application of centrifuge modelling of fluid flow through coarse soils becomes more complicated due to the difficulties and uncertainties to relate the model to the prototype and to satisfy similarity rules. The flow through larger particle-size media is more susceptible to overcome Darcy's conditions in a centrifuge model. In consequence, the analysis of the limits of laminar flow conditions and the migration between laminar, transitional, and turbulent flows, related to variations of centrifuge gravitational level, is required. Different experimental research efforts have been done around this topic including, among others, the work of Goodings (1994) for predicting the characteristics of flow in centrifuge models using sands, or the work of Khalifa et al. (2000) for determining the scaling laws of water flow through different types of sands. Results of these works include theoretical Darcy's permeability scaling laws and the determination of limits between flow conditions limited to certain types of sands (Garnier et al, 2007).

The experimental work presented in this study is attempted to provide new insights related to flow through porous media in a centrifuge model. A series of saturated flow tests increasing hydraulic gradients are reproduced using a 1.3 m-radius geotechnical centrifuge. The experimental setup is designed to allow precisely controlling the increments of hydraulic gradients and maintain laminar flow conditions at different levels of gravity but not limiting the possibilities to Darcy's flow regime. Hence, variations of permeability can be evaluated for a wide range of increments of self-weight allowing examination and validation of centrifuge scaling laws for this parameter as well as for the limits of laminar flow. The effects of particle size, shape, and porosity are evaluated for direct comparisons with the test results available in the literature. In agreement with Khalifa et al. (2000) and Garnier (2007), preliminary results show that Darcy's permeability increases as gravitational forces are increased. Limit of Darcy's flow and relationships of Reynolds number and friction factor are presented for various characteristics of porous media.

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Experimental investigation of pore pressure development in static liquefaction induced failures in saturated sand

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Pore pressure development in sand layers can trigger instability and failure of earth structures. Static liquefaction is one of the most common consequences of instability wherein pore water pressure increments leads to significant decrease in the effective stresses and the soil matrix behaves like a liquid at the failure state. However, there is an ambiguity in definition of the static liquefaction and linking it to a number of fundamental features such as soil properties, effective stress levels and stability of particle arrangements in the soil matrix [1, 2, 3]. Most of the researchers believe that sudden increment of the pore pressure at the onset of failure is a consequence of collapse of the metastable particle arrangement of the soil [3]. In this study, the generation of excess pore pressure in the soil body is experimentally simulated in submerged sand slopes with various initial densities subjected to monotonic loading. The experiments are performed in a unique large scale testing device, so called liquefaction tank (Figure 1). In addition, the results of experiments are compared with those of finite element numerical simulations.

Fig. 1: Static liquefaction in loosely packed sand slopes.

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Physical modeling of sinkhole development around damaged pipelines

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It is very likely that a sinkhole or crater is developed around a leaking/damaged pipeline that is buried in soil. The risk associated with this undesirable phenomenon can be very high especially in urban environment where a network of underground pipelines exists (Rogers et al. 2008). Hence, it is of paramount importance to understand the mechanism of sinkhole development around damaged pipelines in order to provide practical recommendations for preventing catastrophic consequences of pipeline damage.

The development of sinkholes around damaged buried pipelines is classified as a soil-fluid interaction problem which deals with large deformation and fluidization of soil around the damaged area (Alsaydalani 2010). In this study, we aim to provide a deeper understanding of the hydro-mechanical process that leads to the onset of sinkhole development inside sand. To that end, small-scale laboratory experiments were performed on fully saturated samples of silica sand with different initial relative densities. The sand samples were prepared inside a transparent cubic container with Plexiglas walls. A nozzle was embedded at the bottom corner of the container to discharge an upward flow into the sand sample. The discharge was generated through the controlled application of hydraulic gradient in the sample. Two high resolution digital cameras were utilized to take sequential images from the soil at two transparent sides of the container during the discharge process. The Digital Image Correlation technique (DIC) was used to analyze the images for quantification of soil displacement and deformation. The attached figure shows an instance of the sinkhole development inside a dense sand sample. The results showed that the soil failure at the onset of sinkhole development is highly dependent upon the initial state of the tested sand samples. This presentation aims to elaborate the findings of these laboratory simulations.

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Pore water pressures in soil due to freezing/thawing cycles

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In cold areas with major seasonal freezing and thawing periods, features such as soil heaving and thaw consolidation are examples of concern when working with soil in infrastructure. When fine grained granular soils freezes there is expansion of the volume due to phase change of pore water. If water is available beneath the frost front and an open system freezing can be considered, there can be additional water uptake due to suction. When this additional water is freezing, horizontal ice lenses are generated at the frost front. Correspondingly, the soil expands further and the ground surface heaves.

When the soil is thawing, the ratio of generation versus expulsion of excess water determines whether there is generation of excess pore water pressure followed by development of settlements during the additional consolidation. During thawing the frozen soil is acting as a closed boundary and the drainage is only possible in one direction (upwards). As soon as all frozen soil is thawed, there is drainage downwards as well, which enhance the consolidation rate.

Since pore water pressure has a big impact on many structures, the pore water pressure regime (and its development in time) is important to understand not only in serviceability states where the thaw consolidation corresponds to settlements but also for stability analyses where an eventual excess pore water pressure might be crucial.

The freeze-thaw behavior is studied here for a soil deposit in northern Sweden. The average yearly air temperature is 0.1°C and major seasonal freezing and thawing is present. The soil consists of tailings (mine waste), classified by fraction as sandy silt. The material is stored within soil embankments, where the pore water pressure regime is crucial for their stability.

From several piezometers in the deposit, data indicate seasonal cycles in pore water pressure. The variations are considered not solely to be due to variation in groundwater levels. The measured variations are therefore not yet fully understood. The piezometer tips are located below the maximum frost depth (couple of meters deeper). Every summer there are sudden jumps in pore water pressure levels, which with time decreases and gets back to normal stable values.

In the framework of the study laboratory freezing and thawing tests are performed on soil. From these tests it was shown that when the thaw depth reached the maximum frost depth (i.e. when all soil was fully thawed), there was a significant water flow downwards. The pulse of excess water propagated downwards through the soil. Our hypothesis is therefore that this pulse of excess water is the explanation behind the sudden pore water pressure increase in field.

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Stress Sensitivity of Microfractures on Tight Matrix Permeability and Its Effect on Production

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Productivity of tight/unconventional reservoirs strongly depends on the existence of dense microfractures in the sweep volume of the reservoir. The natural microfractures are usually generated, opened or closed as a result of the stress and strain changes induced by hydraulic fracturing or the subsequent production process. Conductivity of natural fractures is highly sensitive to the changes of stress and strain during production. Therefore, stress dependent permeability of tight rock with natural fractures is one of the important parameters for realistic evaluation of the physical properties and the production potential of tight/unconventional reservoirs. The effect of stress on matrix permeability has been studied in detail in the literature; however, research on the variation of microfracture permeability with pore pressure is limited.

The main objective of this paper is to study the effect of stress-dependent natural-microfracture permeability on the productivity of tight/unconventional reservoirs. First, core samples without fractures were selected and a testing procedure was applied to measure the stress dependent permeability as a function of various combinations of effective stresses. Then, a natural fracture was simulated by splitting a whole core and tested under the same effective-stress combinations used for the cores without fractures. Relationships between the pressure-dependent fracture and permeability were obtained by comparing and analyzing the experimental results. A tight reservoir production model was developed to appraise the impact of pressure-related fracture-permeability change with production performance.

Conceptual cases study indicated that effective permeabilities of tight cores with fractures were more sensitive to confining pressure than pore pressure, that is, 0.5~2 orders of magnitude variation of permeability with confining pressure change, and less than one order for pore pressure change. It was also shown that the effect of pressure-dependent fracture permeability on tight-reservoir production is a function of the matrix permeability, and higher matrix permeability is beneficial to release the conductivity contributions of the fracture. Most of the permeability was lost during the initial stage of production, even though the flow rate was relatively high. Therefore, optimization of the production rate and pressure-drop rate was the key to a higher productivity and economic recovery.

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3D gas sorption studies for in-situ measurement of sub-micron porosity of rocks

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Nanoporosity, i.e. the presence of pores at the nanometer scale, is ubiquitous in both natural and engineered systems that are exploited in the petroleum and chemical industry. These include synthetic porous solids, e.g., zeolites used in adsorptive separations, and rocks that are exploited for the recovery of subsurface oil and gas as well as for geological CO2 storage. With reference to reservoir rocks, recent studies have shown that nanoporosity can have a significant impact on their transport properties [1], and on the rate of chemical reactions at solid-fluid interfaces, e.g., dissolution and precipitation [2]. Accurate description of fluid storage, mixing and reactive transport therefore relies on a thorough characterization of the porosity and its distribution within these complex heterogeneous systems.

The use of imaging techniques has nowadays become a standard approach to characterise opaque porous media non-invasively. X-ray Computed Tomography (X-ray CT) yields three dimensional images with spatial resolutions ranging from a few millimetres (medical X-ray CT) to a few microns (bench-scale X-ray micro-CT). Therefore, even at the highest resolution, only pores with width greater than 1 µm can effectively be resolved. In addition to limiting our ability to study the multi-scale transport processes described above experimentally, this also affects the accuracy of pore-network models that are extracted from these images. Most of the available studies that address this issue consider the use of imaging techniques with higher resolution; for instance, FIB-SEM [3] allows resolving both the extent and interconnectivity of the nanoporosity, however, it tends to be destructive. The so-called x-ray saturation method represents an non-invasive alternative that consists of the subtraction of scans acquired with the pore space saturated with two different fluids, e.g., air and water [4] or with a high-salinity contrast brine [5]. Yet, while the achievement of complete saturation is not easily warranted when pores of nanometer dimensions are present, the use of high salinity may lead to unwanted chemical interactions with the solid.

In order to overcome these challenges, we propose a novel approach that relies on the adsorption of gases at sub-critical conditions. Gas adsorption is a well-established tool for the structural characterization of nanoporous solids and adsorption/desorption isotherms are fingerprints of such systems; common metrics that can be gathered from these measurements include surface area, pore volume, pore size distribution, pore connectivity and fractal dimension. In this contribution, we have extended the work reported in Pini et al. [6] by applying the x-ray saturation method to an adsorbing gas (CO2) to quantify adsorption/desorption isotherms in a bench-scale microCT apparatus. As a first step, we have measured gas adsorption isotherms on two well-characterised commercial materials (zeolite 13X and activated carbon) with nanoporosity in the range 1 nm-100 nm. Results from X-ray CT are in agreement with those obtained using standard probing methods. Most significantly, the new method enables quantifying the spatial distribution of gas adsorption, which can be readily translated into the corresponding distribution of sub-micron porosity. As such, this approach represents a practical method to quantify pore-space heterogeneity across multiple scales non-invasively.

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Capillary rise dynamics of liquid hydrocarbons in mesoporous silica as explored by gravimetry, optical and neutron imaging: Nano-rheology and determination of pore size distributions from the shape of imbibition fronts

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We present combined gravimetrical, optical, and neutron imaging measurements of the capillarity-driven infiltration of mesoporous silica glass (Vycor) by hydrocarbons. Square-root-of-time Lucas-Washburn invasion kinetics are found for selected linear alkanes from n-decane (C10) to n-hexacontane (C60) and for squalane, a branched alkane, in porous monoliths with 6.5 nm or 10 nm mean pore diameter, respectively. Humidity-dependent experiments allow us to study the influence on the imbibition kinetics of water layers adsorbed on the pore walls. Except for the longest molecule studied, C60, the invasion kinetics can be described by bulk fluidity and bulk capillarity, provided we assume a sticking, pore-wall adsorbed boundary layer, i.e. a monolayer of water covered by a monolayer of flat-laying hydrocarbons. For C60, however, an enhanced imbibition speed compared to the value expected in the bulk is found. This suggests the onset of velocity slippage at the silica walls or a reduced shear viscosity due to the transition towards a behaviour typical of polymer-like flow in confined geometries. Both, light scattering and neutron imaging, indicate a pronounced roughening of the imbibition fronts. Their overall shape and increase in width can be resolved by neutron imaging. The fronts can be described by a superposition of independent wetting fronts moving with pore size-dependent square-root-of-time laws and weighted according to the pore size distributions obtained from gas sorption isotherms. This finding indicates that the shape of the imbibition front in a porous medium, such as Vycor glass, with interconnected, elongated pores, is solely determined by independent movements of liquid menisci. These are dictated by the Young-Laplace pressure and hydraulic permeability variations and thus the pore size variation at the invasion front. Our results suggest that pore size distributions can be derived from the broadening characteristics of imbibition fronts. [1]

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Characterization of a CO2-saturated porous rock using electrical impedance spectroscopy

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Electrical impedance spectroscopy (EIS) has been performed on a Bentheimer sandstone, which is saturated repetitively with either CO2 or NaCl solution, to monitor the CO2 front propagation. The EIS response is captured in time using a multi-electrode array with linearly spaced electrode pairs. The experiments have been conducted under realistic reservoir pressure-temperature conditions (P=80bar, T= 43°C). Both magnitude and phase spectra of the impedance show a high sensitivity to CO2 injection in the pore spaces.

We demonstrate that the measured impedance of a CO2– or electrolyte-bearing porous sandstone can correctly be modeled by three impedances in series [Kirichek et. al, 2016]. Each of these impedances can be derived by solving a set of electrokinetic equations, and they correspond to different polarization phenomena: electrode polarization (EP) at low frequencies, bulk polarization at mid frequencies (kHz), and pseudo-inductance effect at higher frequencies. EP is correctly predicted in our case using the model presented by Buck (1969) for all investigated concentrations. The bulk contribution that we derived can be accounted for with no adjustable parameter in the case of fully electrolyte-saturated pores when all material properties (porosity, salinity, dielectric constants) are known. We considered the “effective porosity” for some electrode pairs close to the core ends, so as to account for the fact that the core is not properly saturated in electrolyte at these positions, see Fig.1.

As expected, the obtained porosity values differ only by a few percent between electrode pairs. These values for effective porosity were used in subsequent estimation of model parameters during CO2 injection.

The pseudo-inductance effect that we observed can be modelled using one adjustable parameter in case of fully electrolyte-saturated pores, when all material properties (porosity, salinity, dielectric constants) are known. This parameter is linked to an additional conductivity in the neighbourhood of the electrodes in our model. This parameter is then kept fixed in subsequent model-parameter estimation.

When the core is gradually filled with CO2, replacing an electrolyte of a known concentration, it was possible to fit the bulk contribution using the CO2 saturation Sw^n as the only variable (Sw^n = 1 for fully electrolyte-saturated pores and Sw^n = 0 for fully CO2-saturated pores), see Fig.2. Fig. 2 shows Swn values obtained from the best-fit model for the measured complex conductivity. The root-mean-square error is 3.3% and 20% for |σ| and phase, respectively.

Finally, we checked if it was possible to fit the data using both Swn and salinity as variable parameters (porosity and dielectric constants being known). This was indeed possible, as the simultaneous fit of the bulk polarization and pseudo-inductance effect yielded a unique set of parameter values.

We demonstrated that the propagation front of CO2 can be monitored using EIS, at realistic reservoir conditions, and that the model we propose can be used to estimate both salinities and CO2 saturations in the reservoir rock.

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Electro-Kinetic Control of Wettability in a Micro-Fluidic Channel

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The hysteretic relationship between capillary pressure (Pc) on saturation (S) has been shown to be a projection of a higher-dimensional surface that depends on interfacial area per volume (IAV) as the additional state variable. Most studies that validate the capillary-pressure–saturation-IAV relationship are performed on 2D micro-models or cores where scanning is performed in pressure and not in saturation. We have developed an EWOD technique (electro-wetting on dieletric) to internally manipulate fluid saturation to determine the effect on externally measured pressures. EWOD is a technique that uses electrical voltage to alter the wettability of a dielectric material and to create a pressure difference to merge and transport fluids on the material. Our previous experiments demonstrated that application of 0 to 424 V to a droplet of 1 M KCl resting on a PDMinisymposium -surface resulted in a decrease in contact angle from ~120˚ up to 45˚. In this study, EWOD in a sealed micro-fluidic channel was used to determine the effect of EWOD-controlled surface wettability on saturation and externally measured pressures. The sealed micro-fluidic cell consisted of a PDMinisymposium wedge-shaped channel with an entrance width of 0.5 mm and an exit width of 1 mm. The channel length was 2 mm, and had a depth of 0.6 mm. The PDMinisymposium channel was attached to an aluminum plate that served as the ground electrode. An ITO slide coated with PDMinisymposium formed the high voltage electrode and was used to seal the micro-model. When no voltage was applied, a hysteretic capillary pressure and saturation relationship was observed. 636 V was applied to the second electrode to change the wettability of the PDMinisymposium channel. Based on multiple measurements, the externally measured pressure difference that occurred from manipulation of the contact angle by EWOD, ranged from Δp = 250 to 300 Pa. An estimate of the expected pressure difference caused by a change in contact angle can be determined from $\Delta p=2\gamma lv/d(\cos\theta'-\cos\theta 0)$, where γlv the interfacial tension between the liquid and the vapor, d is the aperture of the channel, θ' and $\theta 0$ are the contact angle after and before applying voltage. The calculated Δp was ~280 Pa. Variations in the measured and theoretical values of Δp are attributed to the roughness of the channel and the difference in contact angle for surface experiencing EWOD and those that do not. Only the surfaces perpendicular to the electrical field exhibit a change of surface wettability. EWOD provides method to assess the contributions of wettability to the fundamental physics of immiscsible fluids and film behavior in analog porous media. Acknowledgment: This research was supported by the National Science Foundation (1314663-EAR).

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Study of surfactant loss at rock-liquid interface in Enhanced oil recovery

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Surfactant flooding is one of the mechanism used to enhance oil recovery from the rock reservoirs. Surfactants mainly reduce interfacial tension, increase oil mobility thus allowing better displacement of oil by injected water. One of the main challenges in this process is the loss of surfactant due to adsorption on reservoir rocks [1]. The first adsorbed layer of surfactant is mostly governed by electrostatic attraction. Once this first adsorbed patch forms on the surface, a second layer of surfactant may be adsorbed by surfactant tail-tail hydrophobic interactions at high surfactant concentrations. Both these interaction would be affected by the salt type, salt concertation and pH of the injected solution. We use atomic force microscopy and optical reflectometry[2] to study surfactant adsorption under various brine conditions. AFM force spectroscopy results shows that the adhesion between silica-silica surface s higher in presence of divalent ions compared to monovalent. Also, the magnitude of adhesion increased in presence of surfactant. Further, Reflectometry measurements reveal the extent of surfactant adsorption in presence of monovalent and divalent ions. Both the polar head group of anionic surfactant and the silica substrate are negatively charged under aqueous solutions. Hence the adsorption is mediated via ion bridging mechanism[3]. This adsorption can be reduced by a pre flush of anionic polyelectrolyte which adsorbs strongly in presence of the salt ions[4] and hence repels similarly charged surfactant molecule[1].

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Systematically quantifying micro-emulsion structures using (Spin-echo) Small Angle Neutron scattering

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With the combination of SANS and SESANS neutron scattering techniques, a systematic study has been done in order to quantify the change in structure type and size in micro emulsions. With decane, dodecane and pentadecane as model oils (individually studied), varying either the salinity or co-solvent concentration, clear trends have been observed. For the salinity scan, the phase transition from O/W droplets (44 nm diameter) to bicontinuous to W/O droplets was clearly visible. Furthermore, increasing the co-solvent concentration at optimum salinity from 1%wt to 5%wt showed a significant decrease in the bicontinuous domain sizes. In addition, dynamic SANS measurements have been carried out with a rheometer as sample environment. Change in structure at increasing shear rates has been observed for samples consisting of all three phases (oil, water, micro emulsion).

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Body fluid absorption at the component level and implications on composite performance

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Consumer products absorb body fluids to prevent leakage and to promote physical comfort during use. Nonwoven fabrics made of various natural fibers and synthetic fibers are used to manage the movement and storage of fluid in these products. Changes in porous structure from deformation during wear and interactions of the fluids with the materials occur throughout the life of these products. Changes in uptake of fluids at the component level, e.g. in the fibers, will modify the porous structure at the composite level, e.g. in the nonwoven fabrics, that contain various combinations of these fibers. These changes differ depending on the type and amount of body fluid present. This paper will explore the connection between the uptake of various body fluid simulants in various fiber types and how those differences influence bulk of the fabrics at several saturation levels. This knowledge can inform simulation models and will result in better performing consumer product designs. This knowledge also highlights the need for different absorbent designs for the users of absorbent consumer products.

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Cement particle transport through sack paper

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Paper is one of the most versatile man made materials. Paper is used for packaging, writing, printing, and hygiene to mention just a view. For all these different uses of paper different properties of the material are desired. Packaging paper used for cement bags impressively illustrates that paper is one of the very view materials capable of offering apparently opposing properties in one material. Cement bags are filled in a gas stream with 80% gas and 20% cement within about three seconds. Therefore, (i), the bags need the necessary strength to withstand the pressure difference and at the same time, (ii), the porosity needs to be high enough to let the gas go through, while being, (iii), low enough to keep the cement particles inside the cement bag. With the advent of ever smaller particles in the cement mixtures (additives), the requirements on the pore structure of paper become increasingly stringent. Our work aims at devising numerical simulations that are capable of providing criteria for the required pore structure when considering a given cement composition. The crucial steps are (i) to provide representative pore structures of paper for transport simulations and (ii) to employ a transport model being capable of a multicomponent flow description, i.e., of the gas-cement-additives stream. As a first step, we have analyzed the network structure of a sheet of paper made from soft wood kraft pulp. Figure 1a shows the network structure measured using a µCT (x-ray computer tomography) of the paper before filling with cement. Figure 1b shows the same paper after it has been filled in an industrial setting. It is clear from figure 1a,b that the cement particles are visible in this experiment. However, µ-CT does not allow to differentiate whether the seen particles are single cement particles, or agglomerates from smaller additives added to the cement mixture. We attempted elemental analysis via X-ray fluorescence to obtain additional information on the nature of the particles. To extract the pore structure from the µ-CT data, there are two conceptually different approaches: The most straightforward is to take the void space using a threshold algorithm.[1] However, to capture the properties of the pore structure, it is promising to map the pore network into an augmented graph [2], i.e., a mathematical model comprising the position, size, and shape of the pores as well as their interconnections. Such models allow to (i) swiftly analyse the pore network in terms of porosity, tortuosity, and constrictivity [2] and (ii) construct representative void spaces with pre-defined properties. Realizing that the gas-solid phase flow comprises solid particles with a wide size distribution, we discuss the requirements for a transport model that suitably considers the flow of multiple components, particle-particle and particle-pore wall interactions, and a possibly dynamic pore network due to pore clogging.

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Dynamic pore-network modeling of imbibition in paper coating layer

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Ink spreading and penetration in paper coating layer mostly determine the printing quality [1-4]. Considering size and complex geometry of paper domain, dynamic pore-network modeling is a promising option with acceptable computational costs [5]. In this work, paper coating layer structure reconstructed using FIB-SEM[6] was used to construct the pore network. A single-phase dynamic pore network model was developed for primary imbibition process. This pore network code can be applied to find effects of different pore network structure, coating layer chemical properties and ink composition, on spreading and penetration of ink in coating layer.

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Liquid Absorption in Porous Media Studied by Automatic Scanning Absorptometer

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Over the years, fluid penetration in porous systems has been studied for various industries and applications. The printing industry is one of these industries which attaches great importance to the understanding of ink penetration into paper. Especially, in the inkjet industry, ink absorption is closely related to print quality and print robustness. Therefore, understanding of liquid and ink absorption is very important and requires understanding of both ink and media characteristics, as well as ink-media interactions.

The dynamic process of liquid and ink penetration into paper plays an important role at different length and time scales ranging from nanometer up to millimeter scale and from milliseconds up to days. There is a limited amount of measurement techniques available that allow for quantitative measurements in a space and time resolved manner. In this study, liquid penetration into porous media has been investigated using an automatic scanning absorptometer (ASA) setup which provides quantitative information about the liquid absorption (transferred liquid volume, (TLV/V)) as a function of time (t) on time scales of 10 ms up to 10 s.

Research was focused on the understanding of penetration of well-defined (homogenous) liquids applied on well-defined porous media. According to the one-dimensional model based on Darcy's law, the volume uptake per unit area is related to media parameters (average pore diameter D, tortuosity \tau, porosity \epsilon, contact angle \theta) and liquid parameters (surface tension \gamma, viscosity \eta). The applicability of this theory has been reviewed by testing experimentally the absorption behavior of mixtures consisting of water, glycerol and hexanediol in porous Al2O3 disks and PVDF membranes having well-defined media parameters.

We have found that the results of the liquid absorption experiments on Al2O3 disks can be mapped on a master curve by scaling with media (D) and liquid parameters (\gamma, \eta) leading that no specific media - liquid interactions are presented and results are in agreement with Darcy's law (Ref1) (see Figure 1).

Furthermore, ASA measurement have been done on polyvinylidene fluoride (PVDF) membranes having thickness values (100 to 200 µm) and porosity values comparable to uncoated paper (50 to 70 %). The absorption behavior of water-glycerol in PVDF membranes can be described by an one-dimensional model which is based on the modified Lucas-Washburn model (Ref2). Different behavior was observed for ink penetration where higher absorption speeds were found in comparison with water-glycerol mixtures. The latter can probably be related to a wetting effect caused by interactions between (specific) ink components and the PVDF. The ink penetration behavior scales with D and agrees with the modified Lucas-Washburn model (see Figure 2).

In the end, this study has led to a better understanding of the ASA setup. It has been shown that the ASA setup provides reliable data where the absorption of simple homogeneous liquids on well-defined porous media can be physically explained. This is an important driving force for more research particularly on a better understanding of liquid and ink penetration into paper.

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Pore scale study of hydraulic properties of uncoated paper

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In this study, the three-dimensional structure of fibrous layer of an uncoated paper was reconstructed using images obtained with a µCT scan, with a relatively high resolution of 0.9 µm. Image analysis resulted in pore network of the paper, the domain was used to determine porosity and pore size distribution of the fibrous slayer. Representative elementary volume (REV) was determined by examining values of porosity and permeability obtained for increasingly larger domain sizes. We found the REV should include the full thickness of the paper (150 µm); thus, a cube of 400*400*150 µm was found necessary as the REV. The determined REV size was also checked to be representative for capillary pressure-saturation (Pc-S) curve by obtaining primary imbibition curves for various domain sizes. Doubling REV size in the layer thickness direction had no effect on Pc –S curve. We also investigated the directional dependence of Pc- S curve. We changed position of the wetting and non-wetting reservoirs and placed them in different directions around the REV domain and obtained Pc-S curves. There was no significant difference between Pc- S curves that were obtained. Compression of layer less than 30% had very small effect on flow condition of the layer. We obtained images of water containing fluorescent salt flowing into paper using confocal laser microscopy. We observed that water penetrated fibers and seeped on their surfaces ahead of the main wetting front.

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Porous paper – ink interactions: a spectro- and microscopic view

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The liquid transport in porous paper is an important and actual subject in printing industry. It is well established that both the surface and internal structure of paper influence considerably the liquid penetration mechanisms. Therefore, information concerning the porosity, as well as, the pores‘ dimensions and shapes is needed for a better understanding of the involved processes. In this work we present spectroellipsometry (SE) as a method to investigate the surface porosity of the coated paper. The results are compared with those obtained by helium pycnometry and the limits of the SE method are discussed. In parallel, we have used in our study scanning electron microscopy (SEM) to qualitatively analyze the paper porosity: at the surface and in transversal cross-section obtained by ion polishing. The SEM method is used to investigate and compare different types of paper (coated and non-coated). Moreover the effect of liquid penetration into paper is studied using this SEM method by comparing the images of dry and wetted paper. The changes in fibers dimensions as well as in pores shapes are revealed.

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Quasi-Static Modelling of Fluid-Fluid Movement in a Fibrous Medium

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A new model is presented based on the Young-Laplace equation evaluated at a fluid-fluid interface positioned between two cylinders under a given static contact angle. This model is extended to an array of cylinders positioned parallel to each other in an infinite domain. The model is used to find the smallest possible radius of curvature between pairs of cylinders which gives the largest stable pressure. A parallel is made between quasi-static pore network modelling of a drainage event and the presented theory. This results in the main-drainage curve of the pressure-saturation relation for a set of parallel cylinders. An extension is proposed to model the flow of two phases between non-parallel cylinders. Furthermore a solution needs to be found for the discovery of cylinder positions and radii from real world data like CT-scans and imaging

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The essentials of the water based ink - paper interactions

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The world of printing is rapidly evolving and this is largely fueled by inkjet technology. This printing technology offers the flexibility of digital printing at a breakthrough cost price, delivering good print quality. The R&D de-partment of Océ Technologies, a Canon company, is a major player in the development of inkjet technologies for many different applications.

In this work we will focus on the interactions that happen when a droplet of aqueous ink with polymeric particles meets paper substrate. Under-standing the physical processes that define the interaction between this complex liquid mixture (the water based ink) and the porous paper is vital to have prints of high quality. An overview of these processes will be pre-sented: spreading of ink droplets, water evaporation from inks (thin films and droplets), absorption of the liquid component into porous paper, and drying of the printed ink. The influence of both the liquid physical proper-ties and the paper characteristics will be considered. Methods of investigation will be briefly presented, including their strengths and limitations.

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A new method to characterize the 3D-microstructure of frozen apple using X-ray micro-CT

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Fruits are the highly perishable products like most other plant based products. Their microstructure composed of cells of different sizes and shapes, interconnected cell walls and intracellular air space, of again different sizes and shapes. Fruits pose a particular challenge with respect to freezing. During freezing, ice crystals will be formed and distributed over these compartments. In subsequence storage, they are resized and redistributed resulting in microstructure changes. Non-destructive imaging techniques have become indispensable to improve insight in the microstructural changes in fruit tissues during freezing. Here, X-ray micro-CT was used to visualize, characterize and quantify the 3D microstructure and the ice crystal distribution in plant based products. To this end, apple cortex tissue was considered as a model plant sample with a microstructure consisting of cells and intercellular spaces of different sizes and shapes. Apple samples excised from the cortex tissues were frozen under three different freezing protocols (namely slow, intermediate and fast freezing rates) after which the microstructure and ice crystals were imaged by micro-CT coupled with cooling stage. An image analysis protocol was developed to segment frozen phase from unfrozen matrix, with a help of reference samples being pure ice and sugar solutions. The resulting images were used to quantify and compare the pore space, liquid and ice phase among the different treatments.

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A sea ice pore space analysis in terms of 3-d directed percolation

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Sea ice is a porous medium that forms by unidirectional freezing while floating on its own melt. In the initial freezing process sea ice looses salt by convection, which soon leads to salinities of typically 20 to 50 percent of the seawater from which forms. This convective desalination is driven by solute gradients within the bottom regime of sea ice and thus controlled by the microstructure near the freezing interface (e.g., [1]). The convection also shapes the evolution of a pore space dominated by brine channels that are primarily directed in the direction of gravity. The morphology and connectivity of this pore space should thus best be described by a theory that takes this directionality into account. A reasonable approach is thus to analyse sea ice pore space observations in terms of directed percolation. Directed percolation refers to a universality class of models that, within the field of porous media, may describe fluid movement and pore connectivity in one given direction. Although gravity driven convection in porous media has been suggested as one of the first possible application of directed percolation problems [2], there is rather little experimental data and analysis of such type of application [3]. The present study reports on such an experiment that analysis sea ice macroscopic and microscopic pore space observations in terms of directed percolation. In the present experiment natural arctic sea ice samples have been centrifuged at different temperatures and correspondingly different brine porosities, to produce a macroscopic dataset of connected and disconnected pore space. The centrifuged samples were further imaged by X-ray microtomography (XRT) to obtain the 3-d details of characteristic pore scales and connectivity, as well as their variation with porosity. The results can be interpreted in terms of a connectivity phase transition at a porosity of 2%. The critical exponent of the strength of the percolating cluster is obtained to be in the range 0.79 to 0.83, being consistent with numerical predictions of directed percolation that have proposed a value of 0.81 [3]. The results indicate that unidirectionally growing natural sea ice resembles a porous medium that belongs to the directed percolation unversality class, rather then isotropic percolation as argued in earlier work for the same ice type [4,5]. The porosity threshold of 2% is considerably lower than the frequently cited value of 5% [4] that has been supported by an earlier X-ray tomography study [5]. Our pore scale observations near the threshold indicate that this earlier estimate was limited by spatial resolution, supporting that our estimate of the critical porosity is more feasible and robust.

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Analyzing Brine Channel Morphology in Sea Ice using X-Ray Micro-Computed Tomography

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As the character and dynamics of sea ice change in a rapidly changing climate, it is critical to have a detailed understanding of the fine microstructure of sea ice. Advanced in x-ray micro-computed tomography technology have enabled non-destructive three-dimensional analysis of the brine channel morphology with resolution down to several microns. In this study, we examine both first-year and multi-year ice cores collected from the Ross Sea, Antarctica. By utilizing a cooling stage during scanning, samples were imaged at their in-situ temperatures. The air, brine, and ice phase were each segmented for morphometric and topological analysis. We found a cube measuring 3.75 mm on edge to be the representative elementary volume for all metrics. We observed all samples to contain vertically oriented and mostly cylindrical brine channels, with increasing branching and connectivity observed at lower depths. Air pockets were found to be mostly spherical in shape, except vertically oriented in multi-year ice.

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Characterization of sea ice porosity as a function of temperature in first year sea ice using micro CT X-ray tomography

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Characterization of sea ice porosity as a function of temperature in first year sea ice using micro CT X-ray tomography

Sea ice is a porous medium consisting of pure solid ice matrix and brine and air inclusions. The distribution and chemical composition of these inclusions are temperature dependent. The porosity of sea ice is controlled by the volume and distribution of brine and air inclusions. Sea ice porosity has a strong influence on sea ice physical properties (optical properties and radiative transfer) and biogeochemical processes (transport of solutes and gas); however, there is no fast and accurate methodology to study their spatial distributions, sizes and shapes. A micro CT-scan (Sky scan 1147) placed in a temperature-controlled laboratory providing image of 24.389nm3 voxels (0.029×0.029×0.029mm) is used to assess the porosity of first-year columnar and granular ice. Natural sea ice from Young Sound, Greenland and artificial sea ice grown at the Sea ice Experimental Research facility (SERF, University of Manitoba) previously stored at -25C, were successively warmed to -15C, -10C, and -5C and subsequently cooled to -10C and -15 C. At each temperature step, we realize a morphometric analysis of the brine and air inclusions using CT-imagery analysis. Preliminary results show substantial differences in the spatial distribution of brine and air inclusions between granular and columnar ice. CT-derived brine volume fraction compared well ($R2 = 0.84$, $P<0.01$) to brine volume fraction computed using the state equation of Cox and Weeks [1983] for sea ice temperature lower than -5C. Successive scanning sequences show that for a given temperature sea ice recovers its brine porosity after cooling and/or warming, lending credibility to ex situ analysis of sea ice microstructure at in situ temperatures.

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Densification of Antartica firn by oedometric test under X-Ray micro-tomography

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The depth at which gases are trapped in the ice is dictated by the firn to ice transition. This transition, also termed close-off, is of paramount interest for climate studies. Entrapped air provides composition information of gases that are much younger than the surrounding ice. A precise and reliable relation between firn depth and gas age is still lacking, although it is a necessary condition to understand better the on-going climate change as well as to relate historical climate variations to greenhouse gas emissions. Densification of snow to firn and then to ice under its own weight is thus an essential phenomenon in glaciology. [Rolland du Roscoat et al, 2011] has shown that dry snow can deform by intra-granular strain due to dislocation movements. Although snow densification in Antarctica may originate from various mechanisms such as grain rearrangement, sintering and dislocation glide, in this study, only the last one was first investigated to dissociate the effects.

Firn samples, extracted from Dome Concordia ice core in Antarctica are studied by X-ray micro-tomography. The crystallographic evolution of the c-axis (ice has an hexagonal structure) is also investigated for the same depths. Both results are compared with oedometric experiments performed in a cryostatic cell with controlled displacement. Sample densities range from 0.78 g.cm-3 to 0.87 g.cm-3 and are deformed with strain rates of about 10-5-10-6 s-1. Oedometric mechanical tests emphasize the strong anisotropy and viscoplastic response of firn, with negligible diffusion phenomena. This set-up allows a clear decoupling of diffusion mechanisms (i.e. grain growth) and viscoplastic mechanisms in the densification process. Finally, 3D characterization gives the possibility to follow in-situ porosities and to relate them to the different steps of pore closure in a snow cover. This work also aims to compare the lock-in depth, zone and close-off depth that are determined with climate markers, with physical and morphological parameters.

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Density measurements of young sea ice - a comparison of μ-CT imaging technique and hydrostatic weighing

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Mechanical properties of sea ice are strongly correlated to sea ice parameters such as density, temperature, salinity and porosity. The present study addresses sea ice density evaluation. A frequently applied method to perform density analyses is the evaluation of volume and mass. This approach may give high inaccuracy, as dimensional sample characterization bare a source of error.[1] Two alternative methods were applied and compared. Both methods were applied to young sea ice samples from the Arctic, collected through spring 2016. One approach relies on hydrostatic weighing with para

ffin. Therefor mass of the sample (Mair), mass of the submerged sample (Mpar) and paraffi

n density(ρ par) were evaluated to calculate the sea ice density. The second approach is based on non-destructive X-ray computed micro tomography (μ-CT) scans. The imaging technique is based on the diff
erent X-ray absorption of matter, represented in 3-dimensional images of grey levels. μ-CT scans reveal the 3-dimensional interior and micro-structures of sea-ice (Fig.1). Images were analysed in two ways to estimate density: (i) Conversion of the average grey-level value into a density estimate. (ii) Segmentation into grey values representing air, ice and brine voxels, followed by density determination. Uncertainties of the diff
erent approaches are compared and spatial (horizontal and vertical) and temporal density variation in young sea ice are discussed.

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Ice crystallization in porous rock: the use of X-ray micro-tomography, aims and challenges

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Frost weathering is considered as a major cause of rock damage in humid and temperate to cold climates. Over the last century, different theories on frost weathering of natural stone have been postulated both in a geomorphological context as in the built environment. After the emergence of laboratory X-ray micro-tomography at the end of the nineties, this technique has been used to study rock damage due to frost action (e.g. Ruiz de Argandona et al., 1999; Dewanckele et al., 2013). More recent laboratory developments in fast, continuous X-ray micro-tomography (dynamic CT), open up new possibilities to study the damage process itself (e.g. De Kock et al., 2015). In-situ freeze-thaw cycling of partially saturated limestone, monitored with dynamic CT illustrates the relation of fracturing to the spatial distribution of water to the pore network. Now the question rises if dynamic CT can experimentally resolve the conventional theories based on thermodynamics or experimental measurements using other proxies. One of the challenges here is the distinction of water and ice within a porous rock using X-ray micro-CT, preferentially during the process of phase transition. As this is not possible using conventional grey value discrimination (Fig. 1), other proxies or experimental approaches should be explored in combination with the X-ray scanner equipment. Experiences from other fields or the unconstrained in-situ ice crystallization using X-ray micro-tomography could provide new ideas to tackle this question.

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Interfacial water films observed in gas hydrate-bearing porous matrices effecting wave attenuation modelling

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Accurate mapping of gas hydrate-bearing sediments is of great importance due to two main reasons i) its potential as an energy resource [e.g. Collett and Ladd, 2000] and ii) its potential as a driver for geohazards, namely as a contributing factor for global climate change [e.g. Kvenvolden, 1993] and large submarine landslides [e.g. Nixon and Grozic, 2007]. Gas hydrates are icelike structures forming in a required pT-stability zone – the gas hydrate stability zone. This zone is present in deep sea marine environments and in sub-permafrost sediments. Global warming may trigger hydrate dissociation and therefore destabilization of non-consolidated deep sea sediments at the continental margin. For these reasons it is necessary to find a way to detect not only large hydrate deposits but also hydrate that is distributed in the sediments in a dispersed manner. In this study we used synchrotron-based X-ray computed micro-tomography to resolve the pore space of synthetic samples containing various amounts of gas hydrate. The experimental investigations were conducted at the Swiss Light Source of the Paul Scherrer Institute, where synchrotron micro-tomography allowed us to obtain 3D data on the submicron scale [Chaouachi et al. 2015, Sell et al. 2016, Yang et al. 2016]. In Figure 1 the representative results of the synchrotron experiment are shown. One of the aims was to observe a thin interfacial water layer which is located between the quartz grains and the gas hydrate. Sediments containing hydrates in the pore space are known to show seismic attenuation anomalies in field studies. Currently these anomalies cannot be fully explained whereas squirt flow mechanisms on the microscale are considered to give a reasonable explanation. However, until now, the presence of an interfacial water film in the pore space was only speculated but has not been observed. With the new evidence that such water films exist (Figure 2), new conceptual models must be considered and accompanied of numerical simulations to yield the effective elastic properties of hydrate bearing-sedimentary matrices as well as a better understanding about the predominant attenuation mechanism in these materials. For this, we present our new approach on wave attenuation modelling and our latest results.

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Radiative characterization of morphologically complex multi-scale media - Application to snow with agglomerated soot impurities

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The radiative characterization of heterogeneous media with complex morphologies on multiple scales is of interest in a variety of research areas such as solar energy conversion processes or snow pack [1]. An in-depth understanding and decoupling of the multi-scale morphological effects, bulk material properties, and operating conditions, on the macroscopic behavior provides pathways for multi-scale morphology engineering for improved application performance. We introduce a computational multi-scale methodology for the characterization of the spectral radiative transport in heterogeneous media with complex morphologies on two distinct scales characterized by size parameters (i.e. diameter/wavelength) significantly above and below one. The methodology incorporates the exact morphology at the various scales (obtained by computed tomography and modeling) and utilizes volume-averaging approaches with the corresponding effective properties to couple the scales. At the macroscopic scale, the volume-averaged coupled radiative transfer equations are solved [2] utilizing i) effective radiative transport properties obtained by direct Monte Carlo simulations at the medium scale (mm range) [3], and ii) averaged bulk material properties obtained at the small scale (submicron scale) using Lorenz-Mie theory and discrete dipole approximation (DDA) calculations [4]. The method exemplified to porous snow containing agglomerated soot impurities and validated with experimental data from Hadley et al. [1]. The results show a significant reduction of the calculated reflectance (Graphic 1) and transmittance, and increase of the absorptance of soot contaminated snow compared to pure snow. The exact morphologies in different scales do have significant impact on the discrete and continuum-scale radiative properties. Snow with bigger ice grain sizes showed more sensitivity to the morphological characteristics of the soot impurity (compactness, size, volume fraction and optical properties of the agglomerate). In general, soot in compact aggregates tends to show lower absorption efficiency but higher scattering efficiency than soot in chain-like agglomerates. A quantification and decoupled understanding of the morphological effect on the radiative transport is achieved and a significant influence of the dual-scale morphology on the macroscopic optical behavior is investigated.

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Real time 3D monitoring of frost damage in porous building materials

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At middle to high latitudes, frost weathering is one of the main causes for degradation of porous building materials. Therefore, during the last century, a lot of effort was put into assessing and quantifying the damage caused by ice crystallization through frost-thaw cycle and continuous freezing experiments (Matsuoka and Murton, 2008). However, to make a correct assessment of the damage, it is important to have a good knowledge on the acting damage mechanisms and how it translates to a pressure build-up in the pore space of the material. Several theories were deduced concerning the stress build-up, such as the hydraulic pressure theory of Powers (1945) and the osmotic pressure theory of Powers & Helmuth (1953). The capillary growth pressure theory of Everett (1961), however, is nowadays accepted as the most likely damaging mechanism. Nevertheless, direct evidence that reveals the damage mechanism is still lacking. Multiple approaches have been exerted to deliver this evidence, but imaging by using X-ray micro computed tomography (µCT) was only applied limitedly. The capability of visualizing the freezing process in three dimensions was exploited recently and showed great promise for further research (De Kock et al., 2015). Depending on the structure and connectivity of the pores, different damage mechanisms could be acting. Natural building rocks tend to have an accessible open pore structure, whereas concrete is significantly less permeable and has large gel pores. To make a correct assessment of the mechanism it is required to cover these materials and therefore, three sedimentary rocks (Bentheimer sandstone, Savonnières limestone and a classic Turkish travertine) and two types of concrete with a different water-cement ratio (0.6 and 0.5) were included in this research. By performing dynamic µCT on those samples at the Ghent University Centre for Tomography (UGCT) and using a cooling stage around the sample of interest, high-resolution three-dimensional images during freezing are obtained. Afterwards, two approaches can be considered to deliver the evidence necessary to confirm the damage mechanisms. An attempt directly to monitor the transition of water into ice can be performed. Secondly, the location of the induced micro-cracks within the pores or pore throats can possibly indicate which mechanism has caused them.

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Research of pore ice in frozen sandy soils using X-ray tomography

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Frozen soils are poly-component and multiphase systems. Their microstructure is defined by spatial particle combination of the matrix, ice crystals, various inclusions, unfrozen water and gas component whose size is less than 1 mm. The strength lies of X-ray tomography in its being a non-destruction technique that can investigate the internal structure of the frozen soils. In this work for X-ray tomography investigations were carried out using a SkyScan 1172 X-ray micro-computed tomography system. The availability of Peltye Cooling stage keeps an object at sub-zero temperature during the whole micro-CT experiment allows its using for the investigation of frozen soils. The stage holder temperature was kept at -10° C to avoid ice melting. The most fundamental problem is that, in studying the microstructure of frozen soil using X-Ray tomography is the problem of visualization of main components of the frozen soil. Substances, which typically fill the pores water, ice, clay, etc, have relatively low values of X-ray attenuation coefficients in comparison with those of the solid rock matrix [1]. This makes the phases in the pores almost invisible in X-ray micro-computed tomography experiments. In order to solve this problem in this work the saturating the phases with small amounts of X-ray contrast agents was conducted that allows sufficient improvement in the visibility of these substances in 3D [2]. This method allows us to receive quantitative information on the effect of water content (or moisture content) and mineral composition of the sand soil and identify the main components of their microstructure (such as sand grains, ice-cement and air inclusions). The feature distribution in the pore space of ice and air inclusions was shown on sand frozen samples with different given water content. It is noted, that the regular change of the type of ice-cement occur by raising water content, there is a transition from the film ice-cement to the pore and basal, the size of ice increases (Fig.1). Quantitative characteristics of porosity and pore ice distribution in length sand samples were obtained. The uniform character of distribution the ice saturation for samples with high water content was noted at high-moisture content that apparently related to moisture redistribution at freezing. The results show the great efficiency of X-ray tomography to study the pore ice in the frozen soils.

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Snow isothermal metamorphism: in situ experiment, measurement of interfacial velocities and phase-field modeling for a better understanding of the involved mechanisms

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Once deposited on the ground, snow forms a complex porous material whose microstructure constantly transforms over time. These evolutions, which strongly impact the physical and mechanical properties of snow (e.g. Srivastava et al, 2010; Calonne et al, 2014; Wautier et al, 2015) need to be considered in details for an accurate snowpack modeling. However, some of the physical mechanisms involved in metamorphism are still poorly understood. To address this problem, several investigations combining X-ray tomography and 3D micro-modeling have been carried out over the past decade (e.g. Flin et al, 2003; Kämpfer and Plapp, 2009; Pinzer et al, 2012) but precise comparisons between experimentation and modeling remain difficult. One of the difficulties comes from the lack of high resolution time-lapse series for experiments occurring with very well-defined boundary conditions, and from which precise measurements of the interfacial growth rates can be done.

Thanks to CellDyM, a recently developed cryogenic cell (Calonne et al, 2015), we conducted in situ time-lapse tomographic

experiments on several snow and ice samples under various conditions. We focus here on a 28 h experiment of isothermal metamorphism at -7°C. The non-destructive nature of X-ray microtomography yielded a series of 8 micron resolution images that were acquired with a 2 to 12 h time step. An image analysis method was implemented to estimate the normal growth rates on each point of the ice-air interface and applied to the series obtained. In addition, a curvature-based phase-field model (Bretin et al, 2015) was used on the first image of the experimental series to compute the snow evolution under a pure sublimation-condensation mechanism: the numerical morphologies were then compared to the experimental ones.

The analysis of all the results gives interesting outlooks for the understanding of the physical mechanisms involved in snow isothermal metamorphism. In particular, our measurements confirm the recent observations of Krol and Löwe (2016) that suggest the sublimation-condensation might be predominant over the vapor diffusion mechanism.

Caption of graphic 1: Schematic of CellDyM and simulations of the temperature field within the snow sample. In isothermal conditions, the simulated field is slightly influenced by the outside with temperatures differences of about 0.001°C. All the components situated on both extremities of the snow sample are strictly identical, with the exception of the vacuum pumping system located at the base of the Plexiglas cylinder and the vacuum gauge located in the upper part. For the sake of clarity, the box and the sealing cap of the upper part of the cell are not illustrated.

Caption of graphic 2: Comparison of snow morphologies between experiment and phase-field modeling. Curvature fields are represented on the ice surface. Red corresponds to convexities while green accounts for concavities.

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The Research of Residual Oil Distribution and Micro Contact Relation Based on Digital Rock Technology

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It is very important to research residual oil distribution and the contact relationship between fluid and rock after long-term water flooding for further exploration. The emerging digital rock technology has some characteristics such as nondestructive and repeatability, it can make up for many lacks of general physics experiment. In this paper we established the Micro-CT displacement experiment and obtained the high resolution scanning image of real sandstone sample at different displacement stage. Then the obtained images were preprocessed, segmented and reconstructed using image processing technology in order to make CT scanning image information of multiphase flow conversing to three-dimensional date volume, so we can describe the distribution types and characteristics of oil and water. For the remaining oil with different distribution type, we used some index like the contact angle, curvature and wettability to quantitatively evaluate the micro contact relationship between reservoir fluid and rock. Finally, we analyzed the effect of different water injection multiples, displacement pressure, rock's composition, pore throat size and fluid properties on the remaining oil distribution features and contact relationship. Through the study of this article, we can analyze the reservoir fluid distribution and contact relationship after displacement from the microscopic view, so it can provide the basis for further digging of residual oil.

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X-Ray tomography to characterize entrapped oil in sea ice: how to differentiate oil, brine and ice

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Receding Arctic perennial sea ice and the expected suspected presence of substantial oil and gas reserves in the Arctic are likely to drive an increase of oil extraction and transport throughout the maritime Arctic. Despite a decrease in sea ice extent, Arctic waters remain covered with sea ice, which is a significant hazard for anthropogenic operations most of the year. Sea ice is composed of a network of pores and channels filled with brine encompassed in a matrix of freshwater ice. Porosity serves as an important habitat for microbial communities which support the Arctic food web. At the same time, it can trap a substantial amount of oil in the event of a potential oil spill. Porosity and microstructure evolution in sea ice is dominated by the combination of ice temperature and bulk salinity [1]. During warming events, the brine volume fraction tends to increase, and pores interconnect, leading to a higher permeability. Experimental studies and observations of recorded data show that up to 20% of the ice volume could potentially be occupied by oil in May [2]. We are interested in the linkages between sea ice pore microstructure and the oil entrapped. Sea ice is grown from artificial seawater exposed to the air of a cold room. After the oil release, the ice is sample before and after warming, which simulates the spring melt. Ice samples are observed with a micro X-Ray tomograph to characterize pore geometry and microcomputer. Due to similar density values of the different phases, differentiation between ice, oil, and brine using X-Ray tomography, though possible, is challenging. Automated digital processing remains, even more, complicated to implement. In a recent study, oil entrapment in sea ice is modeled from 3D tomography imagery of a centrifuge sea ice sample [3]. We focus on in-situ oil detection in sea ice and compare different methods to observe oil contaminated sea ice. The sample is cooled down until the brine freeze before centrifugation. Porosity previously filled with oil will appears as empty cavities in X-Ray tomography imagery. Based on previous work, artificial sea water is doped with CsCl to increase the brine density and contrast [4]. Both technics will be applied to enhance oil detection. Optical imagery of thin sections is used to corroborate the analysis at a millimeter scale.

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X-ray nanotomography of sea urchin spines

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The calciferous exoskeletons of marine invertebrates have been optimised by evolutionary processes over millions of years to deter predators and to withstand the enormous pressure of water, while remaining light weight by preserving a high degree of porosity. Understanding the construction principles of this class of organisms is thus not of mere academic interest but can also lead to new design strategies for man-made materials using nature as a template.

In a previous study, we recorded X-ray tomography data on a laboratory source of shells of a sea urchin subspecies and performed finite element simulations (Graphic 1) showing that the shell is made up of a highly porous (up to 70%) structure which behaves mechanically close to an ideal foam [1]. Despite this encouraging result, applying the same approach to the more functionalized parts of the sea urchin, i.e. the spines, is limited because the laboratory instrument's resolution (~1 µm) is insufficient to resolve the much more fine scale morphology of the spines (Graphic 2 inset). Here we present X-ray nanotomography data from beamline BL47XU at SPring-8, Japan [2] with a voxel size of 40.5 nm (Graphic 2). Analyzing these data, we can interpret the spine's core as bundles of cylinders orientated along the spine's axis thus maximizing resistance against deformation in this direction. Occasional crosslinkers between the cylinders help to improve the mechanical stability in the plane perpendicular to the spine's axis. These morphological observations are supported by finite element simulations based on the tomography data and complementary in-situ deformation studies.

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Correlating Mesoporous Microstructures to Bulk Transport in a Fluid Catalytic Cracking Particle

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Fluid Catalytic Cracking (FCC) particles are considered to be the workhorses in oil refineries for the production of an important fraction of propylene, used for plastics, as well as gasoline. The spherical FCC particles have an average diameter ranging from 50 – 150 µm and consist of several components, such as zeolite, clay, alumina and silica. Transport of feedstock and their reaction products through the FCC particles occurs over length scales varying from several tens of micrometers down to sub-nanometers levels, as the final catalytic cracking of feedstock molecules occurs within the zeolites [1]. Hence, the challenge is to quantitatively relate the micro-, meso- and macropore space together with a larger scale spatial heterogeneity of the pore space to the transport efficiency for molecules to and from the zeolite components.

We developed a workflow [2] capable of determining the transport efficiency, or transport ability, of heterogeneous catalysts based on their microstructure. The workflow takes into account the heterogeneity across the largest significant length scale, i.e. up to the size of an entire catalyst particle. The first step maps the overall meso pore space in 2D and in detail in 3D using a Focused Ion Beam – Scanning Electron Microscope (FIB-SEM) [3]. Geometrical parameters (i.e., porosity, connectivity and heterogeneity) are determined from the 3D volumes and used to generate large numbers of virtual 3D volumes. The virtual 3D volumes resemble the sample's pore space characteristics, while being suitable for computationally demanding transport simulations (finite element steady-state diffusion). Next, a porosity-dependent probability function is fitted to data obtained from the simulated transport ability through the virtual volumes. The combination of this porosity-dependent probability function of the transport ability and the measured spatial porosity distribution (determined in 2D) allows for an up-scaling routine that is based on an analogue to electrical resistors [4,5]. The up-scaling routine enables the characterization of the catalyst body at relevant length scales, based on its experimentally determined meso- and macro porosity. An example will be shown for two different types of FCC particles. Based on our analysis, differences in bulk properties can be qualitatively linked to differences in the organization of the pore space.

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Experimental characterization of the organic pore network of source rocks at the nano-scale

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The geometry of the organic pore networks plays a key role in controlling the fluid transport properties of source rocks. Its characterization is challenging because a significant portion is comprised between 0.1 and 50 nm in diameter[1]. This micro to meso-porosity is believed to be responsible for the low permeability, strong adsorption, and non-Darcy behaviour of these geomaterials[2]. It results in reduced hydrocarbons flow, partly accounting for the fast productivity declines noticed in exploitation wells around the globe[3]. In order to improve the accuracy of production predictions, it is paramount to understand the evolution of organic hosted pores in terms of morphology and topology as a function of thermal maturity. An experimental study of the organic matter hosted pores was therefore initiated by coupling BET with electron tomography. Three different formations (Lower Eagle Ford, Marcellus, and Haynesville) containing variable contents of organic material with different thermal maturities have been studied. LEF is thermally immature (oil-prone) whereas MAR and HAY are thermally overmature (gas-prone)[4]. The adsorption isotherms showed a noticeable increase of the specific surface area (As) and, hence, a decrease of the average pore size (rH) as a function of the vitrinite reflectance (VR0), in agreement with the trend observed in North American source rocks[5]. This led to the hypothesis that the transition from oil-prone to gas-prone is accompanied with the closure of meso and macro-pores and the formation of meso to micro-pores. To verify this hypothesis, thin sections of organic material (kerogen and bitumen) were extracted using a Focused Ion Beam. This approach allows comparing the organic hosted porosity at different thermal maturities (LEF / HAY-MAR) as well as different nature of organic material (kerogen/bitumen). The FIB thin sections were then studied by electron tomography. This tomography technique uses a transmission electron microscope with a single axis tilt apparatus that can image pores with radii ranging from 0.5 to 25 nm. A set of image treatments have been applied to the tilt series from the acquisition to the reconstruction in order to have access to the geometrical arrangement of organic pores in 3D. The produced tomograms were then analysed using the public domain software iMorph. The results showed that the pore size distributions and surface areas from aperture map computations, chord length distributions, and surface meshing are in good agreement with the N2 adsorption isotherms. The definition of the minimal geometrical path (tortuosity) from face to face evidenced disconnected porosities according to the x and y directions of the tomograms, and elongated pores that connect both faces in the z direction in all samples. Potential artefacts induced by the acquisition procedure and/or the reconstruction will be discussed. Overcoming these artefacts is fundamental to identify potential connected networks and defining their percolation thresholds, which represents the critical parameter for understanding and predicting the fluid transport mechanisms.

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Experimental investigation on the coupled effect of effective stress and gas slippage on the permeability of shale

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Permeability is one of the most important parameters to evaluate gas production in shale reservoirs. Because shale permeability is extremely low, gas is often used in the laboratory to measure permeability. However, the measured apparent gas permeability is higher than the intrinsic permeability due to the gas slippage effect, which could be even more dominant for materials with nanopores. Increasing gas pressure during tests reduces gas slippage effect, but it also decreases the effective stress which in turn influences the permeability. The coupled effect of gas slippage and effective stress on shale permeability remains unclear. Here we perform laboratory experiments on Longmaxi shale specimens to explore the coupled effect. We use the pressure transient method to measure permeability under different stress and pressure conditions. Our results reveal that the apparent measured permeability is controlled by these two competing effects. With increasing gas pressure, there exists a pressure threshold at which the dominant effect on the intrinsic permeability switches from gas slippage to effective stress. Based on the Klinkenberg model, we propose a new conceptual model that incorporates both competing effects. Combining microstructure analysis, we further discuss the roles of stress, gas pressure and water contents on gas permeability of shale.

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Impact of Clay Mineralogy on Hydraulic Conductivity and Geomechanics of Shale Caprocks

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Shale cap rocks are nature's best hydraulic barrier geomaterials. They are effective seals for underground hydrocarbon bearing formations as well as the CO2 storage formations in carbon capture and storage (CCS) projects. The sealing properties of shale rocks are directly related to its minerals and the internal arrangement of clay and non-clay minerals known as a microstructure. Since shales are predominantly composed of clay minerals, the type and amount of clay minerals contained within the rock are the key factors of its sealing properties. The goal of this study is to gain a better understanding of the how different types of clays behave in a typical CO2 storage reservoir condition. Clay minerals have a layered structure which often carries a negative surface charge. This combination of the large reactive surface area and charge brings complexity in terms of their reactivity to fluids. Therefore, even the same type of clays can have different properties depending on their depositional environment, which was influenced by different fluid properties (pH, T, P, salinity). The same is also true of the exposure of clay-rich rocks to reactive fluids during geologic times as well as under subsurface engineering conditions (nuclear waste storage, injection of waste water and fracking fluids in O&G, and carbon sequestration). For this study, artificial shale rock samples were designed using purified natural minerals in different ratios. These samples allowed us to observe the impact of the mineralogical composition on mechanical properties and obtain a systematically quantified comparison between samples. After re-sedimentation, the samples were fractured and exposed to solutions with different pH / salinities. X-ray Photoelectron Spectroscopy (XPS) was utilized to identify the change in the mineralogical composition while Scanning Electron Microscopy (SEM) was used to obtain the microstructure. The indentation tests were conducted to evaluate the change in the mechanical properties as a result of solid/fluid interaction. Observation in this study indicate: a) a transport and participate of certain types of clay minerals along the fracture surface; b) a reactive transport of dissolved calcium based minerals, which result in occluding micro-fracture flow paths, thereby improving shale caprock seal integrity with respect to leakage risk under CO2 sequestration conditions.

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Lithological variations in the Boom Clay: effect on the porous network and transport parameters

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In Belgium, the Belgian radioactive waste management organization ONDRAF/NIRAS considers Boom Clay as a potential host formation for a geological disposal facility for nuclear waste. Because of the low permeability and the low hydraulic gradient over this formation, solute transport in Boom Clay is dominated by diffusion. Boom Clay consists of different lithological sub-units with a rhythmic alteration of silty and more clay-rich layers, and organic-rich and carbonate-rich layers. From previous work, it is well known that these variations in clay and silt content lead to changes in transport parameters such as hydraulic conductivity (Wemaere et al., 2008) and diffusivity (Aertsens et al., 2005; Bruggeman et al., 2009). In order to extend our knowledge on the effect of clay/silt content on the diffusive parameters (effective (Deff) and pore (Dp) diffusion coefficient and porosity (η)), we performed diffusion experiments with He, Ne, CH_4, C_2H_6 on samples with different clay/silt content. In a second step we tried to identify the petrophysical parameters that influence the diffusion parameters. Therefore, samples were fully characterized through petrographical analysis of thin sections and computer tomography (CT) on several scales and in terms of grain size characteristics and mineralogy.

All samples with elevated silt content were associated with an increased hydraulic conductivity (K). As expected, silty samples also exhibit elevated diffusion coefficients. This effect was observed for the samples oriented parallel (//) to bedding plane, but was less pronounced for the samples oriented perpendicular (⊥) to bedding plane. The geometric factor (G = η x D0/Deff), expressing the influence of pore structure, geometry and connectivity on the diffusion process, is – as expected - smaller for the silty samples. Note further that especially for the // samples, the effect on the diffusion parameters is larger when the size of the molecule increases. For the ⊥ samples, correlations are noted between the geometric factor and the mineralogical composition (2:1 clay minerals and quartz content). Petrographic analyses of thin sections ⊥ to bedding showed a clear difference between the "clayey" and the "silty" samples (Fig.1). In the clayey samples, the quartz grains are homogeneously distributed over the clay matrix, whereas the silty samples are characterized by clusters of quartz grains with inter-particle porosity. After filtering out the zones with a higher porosity in the µ-CT images and reconstructing them in 3D, interconnected (same color) paths with a higher porosity become visible, which can be linked to bioturbations. In the clayey samples, zones with higher porosity are small and randomly distributed

(larger structures are drying cracks). These results support the hypothesis that lithological variations and bioturbations influence the pathways for diffusive transport through the formation to a certain extent.

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Micro-CT imaging and analysis of 3D pore structures in tight rocks and their pore-scale distribution of multiphase fluids after transport processes

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Digital rock technology provides 3D multi-resolution images of rock samples for simulations of transport through their pore space. This rapidly developing capability is especially promising for tight rocks, on which traditional laboratory measurements of transport properties are often problematic. However, tight rocks also pose challenges for imaging and simulation. Developments in 3D imaging of the largely-unknown pore-scale distributions of multi-phase fluids, in preserved reservoir samples or after laboratory experiments, are required to further guide simulations. This paper further extends recent advances in micro-CT imaging and analysis [1-6] to tight gas sandstones and reservoir shale mudstones.

For a set of tight gas reservoir sandstones, small plugs (sub-plugs) of 3-5 mm diameter were micro-CT scanned in the cleaned state and afterwards in a sequence of prepared states, designed to accentuate the X-ray contrast of key features lying below tomogram voxel size (of around 2 micron). In particular, imaging was performed after the connected pore space was saturated with an X-ray dense wetting fluid (diiodomethane, CH_2I_2), and after subsequent drainage by centrifugation in air. Each acquired tomogram was spatially registered to the clean-state tomogram, in order to generate the difference tomogram in which the rock contributions are subtracted to thus highlight the fluid distribution for quantitative segmentation. This analysis provides a 3D map of the porosity (from resolved and sub-resolution pores) per voxel, and of the wetting-phase saturation per voxel at the local capillary pressure. A further contrast-enhanced state was acquired by adsorbing an X-ray dense species to the rock surfaces, which produced a corresponding 3D map of local surface area/volume. After these non-destructive steps, the rock sub-plug was sectioned for acquisition of 2D image mosaics by SEM and SEM-EDS, which were registered to overlay their corresponding virtual section through the sub-plug tomogram. In this way, characteristics of porosity, pore-throat size and surface area from tomographic mapping were point-wise compared and ascribed to the local mineralogy. Examples from tomogram slices are provided in Figure 1.

Micro-CT imaging of the preserved state of reservoir shales cannot directly provide information on the detailed distribution of oil, air and water in place, owing to their tightness and to the similarly low X-ray attenuation of these three fluids. An analogous approach to that described above was used to selectively boost the attenuation of these three fluids. Each shale sub-plug was micro-CT scanned after 1) highlighting of in-place oil, 2) highlighting of in-place oil plus air, 3) cleaning to define the fully empty reference state, and 4) saturation to highlight all connected pore space. Figure 2 shows the registered pair of tomograms of one shale sample before and after brightening of in-place oil. The 3D distribution of in-place fluids from segmentation of the registered tomogram differences was directly compared to the fine-scale morphology and mineralogy of pores, organic matter, grains and clays from 2D SEM and SEM-EDS images. In particular, most of the in-place oil in these samples was strongly associated with calcite and organic matter, while the matrix clays were predominately water-filled and water-wet.

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Microporous rocks: insights from gas adsorption experiments

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Shale rocks contain very narrow pores with nanometer dimensions that are the primary cause for their low (matrix) permeability. These nanopores create intimate fluid-rock interactions that lead to the physical adsorption of gases, i.e. to the trapping of gas molecules at near liquid-like densities attached to surfaces of pores in the material. Understanding the mechanisms of gas sorption in shale rocks is important for several reasons. First, while gas adsorption is a physical process that contributes towards enhancing the storage capacity of shale systems, gas desorption from their tight matrix may be a key factor that limits production rates. Secondly, classic characterization techniques for micro- and meso-porous materials are adsorption-based and therefore rely on the ability to understand fluid behavior and transport under confinement.

Both sub- and super-critical adsorption studies have been reported in the literature to address these aspects, but the picture is still far from being complete. The main reason for this is the intrinsic difficulty in performing these experiments at both sub- [1] and super-critical conditions [2], and in their description, because the interactions between the gases and the main mineral constituents of shale (e.g., clays and organic matter) are quite complex [3], leading to contrasting observations, such as densification and/or depletion phenomena [4].

In this paper, we report results from a systematic investigation on the adsorption properties of shale rocks, by covering a wide range of conditions and by using various samples, including organic-rich and organic-lean samples. The experimental techniques include (i) a Rubotherm Magnetic Suspension balance for the measurement of supercritical CO2 and CH4 adsorption isotherms and a (ii) Micromeritics 3Flex instrument for low-pressure cryogenic adsorption experiments. For the latter, two adsorbates are used, namely N2 (77K) and CO2 (273K), so as to probe fully the microporosity of the adsorbents. Shale samples come from various locations around the world, including major plays in the United States (e.g., Eagle Ford and Utica Shale) and potential plays in the UK (the Bowland Shale). Additionally, to inform the interpretation of results from shale samples, observations are used from reference materials with well-known pore-size structure and compositions, such as micro- and meso-porous adsorbents as well as pure clays.

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Multiscale Characterization of Shale Porosity using multiscale X-ray and electron microscopy

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The analysis of pore size distribution analysis plays a critical role in determining gas storage capacity and fluid transport characterization in shales. Study of the diverse distribution of pore size and structure in such low permeability rocks is withheld by the lack of integrated tools to visualize their microstructure. Frequently the resolution required to image the fundamental structures in these samples comes at the expense of a field of view representative of true subsurface heterogeneity. In this study we integrate multiple techniques to investigate the full pore size range in different sample scales. Modern imaging techniques are combined with routine analytical investigations (x-ray diffraction, thin section analysis and mercury porosimetry) to describe pore size distribution of shale samples from Haynesville formation in East Texas to generate a more holistic understanding of the porosity structure in shales, ranging from standard core plug down to nm scales. Standard 1" diameter core plug samples were first imaged using a Versa 3D x-ray microscope at lower resolutions. Then we pick several regions of interest (ROIs) with various micro-features (such as micro-cracks and high organic matters) in the rock samples to run higher resolution CT scans using a non-destructive interior tomography scans. After this step, we cut the samples and drill 5 mm diameter cores out of the selected ROIs. Then we rescan the samples to measure porosity distribution of the 5 mm cores. We repeat this step for samples with diameter of 1 mm being cut out of the 5 mm cores using a laser cutting machine. After comparing the pore structure and distribution of the samples measured form micro-CT analysis, we move to nano-scale imaging to capture the ultra-fine pores within the shale samples. At this stage, the diameter of the 1 mm samples will be milled down to 70 microns using the laser beam. We scan these samples in a nanoscale X-ray microscope (with a spatial resolution of 50nm) and calculate the porosity of the samples by image segmentation methods. Finally, we use images collected from focused ion beam scanning electron microscopy (FIB-SEM) to be able to compare the results of porosity measurements from all different imaging techniques. These multi-scale characterization techniques are then compared with traditional analytical techniques such as Mercury Porosimetry.

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On the hydraulic conductivity of thin, planar cracks in shale and tight sandstone as a function of shear and normal stress.

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Conductivity of fluids along fractures in rocks is reduced by increasing normal stress across the crack, and this has previously been experimentally verified, but the conventional view that the onset of shear failure along planar cracks enhances fluid flow owing to a small amount of dilatancy has not been unambiguously demonstrated. Fluid flow in cracks is usually modelled from the bottom up, beginning with the 'cubic law' relating flow rate along a parallel-sided channel to its width, then adding complexity due to crack roughness and tortuosity of flow paths, when it becomes difficult to define a crack 'width'. Here we determine experimentally how increasing normal and shear stress affects fluid flow along cracks using an electrical analogy, in which the crack is replaced by a slab of homogeneous material of greater permeability. This greatly simplifies the problem. Hydraulic conductivity (dimensions m3) is crack material permeability x crack width, so that bulk matrix permeability is equivalent to the hydraulic conductivity of a 1 m thickness of material. A crack with the same hydraulic conductivity would be a thinner layer filled with a more permeable material. We used argon gas to measure conductivity of planar cracks in Bowland shale and a higher viscosity synthetic oil for the much more conductive Pennant sandstone. In both cases conductivity is reduced by increasing effective normal stress (over a range of 80 MPa), and conductivity is recoverable during pressure cycling. Shear stress was increased at constant resolved normal stress using servo-control of the pressure system until the onset of frictional sliding. In both cases, at this point the conductivity decreases markedly and permanently, evidently due to the formation of a very thin layer of very fine-grained (10 micron) fault gouge as crack surface asperities are broken through and granulated. The positive normal stress sensitivity of friction stress indicates that there is local dilatancy, but from the point of view of conductivity, this is clearly swamped by the formation of the fine, low conductivity gouge matrix and its compaction. The combination of increasing normal stress and shearing can reduce conductivity by up to 5 orders of magnitude. Presently, we have not accessed any physical conditions, such as sufficiently low effective normal stresses, which might lead to sufficient dilatation to permit an increase in conductivity with incipient shear displacement. These results can impact greatly on approaches to the modelling of fluid flow through rock masses containing crack arrays, necessary for the design of hydraulic fracture treatments, geothermal energy extraction, the design of waste repositories in a range of rock types and the flow of reservoir fluids.

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Pore geometry and connectivity characterization using BIB-SEM and Liquid Metal Injection for better understanding of transport properties in tight rocks

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Evaluation of transport properties in tight rocks such as shales by imaging methods is complex because of the small pores, small pore throats and sample inhomogeneity. Two dimensional BIB-SEM imaging can resolve pores down to several nanometers and map the mineral heterogeneities in representative areas. However, it cannot show the pore connection directly due to the absence of the third dimension. In this contribution we present a routine to obtain a first estimate of permeability from pore geometries acquired by BIB-SEM in representative elementary area. Quantitative pore properties are obtained from secondary electron, backscatter electron and energy-dispersive X-ray spectroscopy image maps by using dedicated image processing algorithms. From the derived pore sizes a first approximate of the permeability can be estimated by applying the capillary tube model, which is a combination of Poiseuille's and Darcy's law. The primary results can be enhanced by information obtained by Liquid Metal Injection (LMI) followed by BIB-SEM. During LMI a fusible alloy is injected into the rock sample at incremental pressure steps forcing the liquid metal into the pore throats filling up the pore bodies. Subsequently in SEM, the BIB polished section reveals the metal filled pores indicating the connected part of the pore space and the permeable layers. By combining our outcomes with experimental data we get a better understanding of the connected porosity, permeability, tortuosity and pore throat sizes. In this contribution we present comparative example studies of several tight rock formations.

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Pore network and permeability of the Whitby Mudstone (UK)

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Shale reservoir potential is largely determined by the connected pore network in the rock, the connection between the pore and the fracture network, and the corresponding total permeability of the rock. Typical pore diameters in shales range from the µm down to the nm scale, with the majority of the pore throats having diameters smaller than 100 nm. We have used a combination of Broad-Ion-Beam polishing and Scanning Electron Microscopy (BIB-SEM), Focused-Ion-Beam polishing and Scanning Electron Microscopy (FIB-SEM) and pressure step decay methods to image the pores and pore network, and measure the permeability of the Whitby Mudstone. The Whitby Mudstone is the exposed counterpart of the Posidonia Shale, present at one to three kilometers depth in the Dutch subsurface, where the Early Jurassic (Toarcian) Shales (Whitby Mudstone, Posidonia Shale, Schistes Carton) in Northern Europe are investigated as possible unconventional sources for gas.

Whitby Mudstone is a heterogeneous clay matrix rich rock (60-80%; clay matrix are all minerals with diameters < 2nm) with a low porosity (He-porosity 1-7%). Measured matrix permeability values for the Whitby Mudstone are in the order of Micro to Nano Darcy and permeability is controlled by microstructural complexity of the samples. The complexity is due to the interplay between porosity and mineralogy, but also due to the exact arrangement of the minerals (grain boundaries), pores and possible micro fractures at different scales. Typical microstructures reveal minerals floating in a clay matrix, with no connected pore pathways for the gas visible at the resolution used for imaging in 2D. Visible BIB-SEM porosity is between 0.5 and 2.5%. FIB-SEM data reveals the pore bodies, connected and unconnected pore networks (3D) present in the clay matrix of the Whitby Mudstone, where visible FIB-SEM porosity ranged between 1.1 and 7.3%. The FIB-SEM data does show that part of the pore networks are connected at the nm-µm scale, indicating that the gas is naturally accessible, but only through a very badly connected pore network.

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Pore structure characterization of a tight oil reservoir by mercury intrusion Porosimetry using different fractal models

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Different from conventional oil reservoirs, tight oil reservoir is challenging to develop due to ultra-low permeability. Nano scale pores and throats combined with micro pores consist of complex pore network, and correctly characterizing the pore structure of tight oil reservoir is of great importance to tight oil reservoir development. This paper investigates the pore structure of a tight oil reservoir from China by mercury intrusion porosimetry using different fractal models. Although fractal theory can effectively describe the of pore size distribution and characterize the heterogeneity of pore structure, there are several different fractal dimension calculation methods using mercury intrusion curves, and different fractal models give different result, which are confusing. This paper applies six different fractal models to characterize the pore structure of tight oil reservoir, including wetting phase model, 2D capillary tube model, 3D capillary tube model, 3D capillary tube model with Washburn Equation, geometry model and thermodynamic model. After that, the fractal permeability model is established to investigate the effect of pore structure on the permeability of tight oil reservoir.

The research result shows that the fractal dimension calculated using wetting phase model cannot correctly characterize the pore structure of tight oil reservoir, and the calculated fractal dimension has no obvious relationship with the petrophysical properties of tight core samples. The calculated fractal dimension using 2D capillary model is generally less than 2, and the fractal dimension calculated using 3D capillary tube model with Washburn Equation is less than that using 3D capillary tube model, and varies between 2 and 3. The fractal dimension calculated using geometry model is close to that calculated using thermodynamic model, but the difference is geometry model reflects the space heterogeneity and thermodynamic model reflects the surface roughness. For the fractal permeability model, when the average pore radius is larger than 0.2 micrometer, the calculated permeability is very close to the air permeability. However, when the average pore radius is less than 0.2 micrometer, the error of calculated permeability increases sharply with the decreasing average pore radius, which means the fractal permeability model needs amended amendment for the ultra-low permeability core samples.

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Prediction of effective diffusion coefficients of mudrocks from pore network fractal data

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Molecular diffusion in low permeability sedimentary rocks is characterized by low transport rates, but it is a ubiquitous process, controlling water-rock reactions, seal capacity or production from tight gas reservoirs. Experiments determining the effective diffusion coefficient in water-saturated shales are rare due to the technical complexities and long time-scales required to obtain steady-state conditions. Plug sizes are usually a few millimetres to a few centimetres in length and it can take several months until steady state conditions are reached. Here we present a model that combines direct measures of the fractal dimensions of the pore network using neutron scattering measurements with analytical models of diffusive transport in capillary bundles (Liu and Nie, 2001; Liu et al., 2004) to predict diffusive transport rates in low permeability rocks. We use small and very small angle neutron scattering measurements, providing pore size characterization over 4 orders of magnitude, to determine the pore network surface and volume fractal dimensions. The model results are compared with actual laboratory diffusion measurements carried out on three different sample sets of different geological provenance, mineralogy, depositional environment and age: Opalinus Shale: All Opalinus Shale samples used in this study were taken from the shaly facies of the Opalinus Clay formation at the Mont Terri underground rock laboratory, St. Ursanne, Switzerland. From a ~2m core section we cut ~1cm disks in 10cm intervals to be used for a number of laboratory tests which have been reported earlier (Amann-Hildenbrand et al., 2015; Busch et al., accepted). Carmel shale: This shale was obtained from a scientific drilling campaign near Green River, Utah. The geological setting and depositional environment was described previously (Kampman et al., 2014; Kampman et al., 2016). For the diffusion experiments using CO2 as a solute we used a plug drilled from a depth of 573 ft (180.7 m) that mainly consists of quartz, illite, calcite and some minor K-feldspar, dolomite and hematite. Boom Clay: All Boom Clay samples used in this study are taken from the ON-Mol1 borehole, drilled in 1997, in Mol, Belgium. In total 5 samples have been used for the neutron measurements and compared to experimentally derived values from (Jacops et al., submitted). Samples are from the Putte, Terhagen and Boeretang members of the Boom Clay formation and can be classified as clayey (ON-Mol-1 84b, 112a, 127b) and silty (48a1, 48a2). The mineralogy is dominated by quartz and illite/smectite with some minor muscovite, kaolinite and K-feldspar. Total clay content varies between 53 and 65 %. Results of this comparison are presented in Figure 1, showing a plot for measured and calculated effective diffusion coefficients on the different mudrocks. Especially when laboratory determined diffusion values were measured parallel to bedding the agreement is remarkably good. When plugs were tested perpendicular to bedding, the fractal models overestimates the measured values by a factor of 5 at most, which, given the large uncertainties in the measured data, we consider to be acceptable. To our knowledge, this is the first

attempt to compare directly a capillary bundle model of tortuous pore networks parameterized using SANS data, with laboratory based diffusion coefficients on the same samples, and for a range of different experimental fluids. In summary, this method has the potential to provide effective diffusion coeffcients for porous materials with nanometer-size pore diameters using a quick, non-distructive method, small samples (1×1cm and a thickness of <0.5 mm), including highly spatially resolved samples, such that spatial variations in the pore network at the core scales can be investigated (e.g. changes with core scale trends in mineralogy or facies).

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Scanning SAXS/WAXS Microscopy applied to organic rich shales to quantify local distribution and orientation of pores and minerals

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The shale microstructure controls flow and transport processes that are relevant for gas storage, radioactive waste disposal and shale gas production. The microstructure however, is heterogeneous across many different length scales, in terms of pore size distribution and mineralogy. It is therefore challenging to represent statistically representative pore networks in shales. Standard characterisation methods either resolve volume averaged properties, or fail to assess statistically representative sample volumes. As a consequence open questions remain about the pore arrangement across the different lengthscales. In the present study we apply scanning small and wide angle X-ray scattering (SAXS and WAXS) microscopy[1,2,3] on organic rich shales. On each sample a series of scans are taken along a raster, using a microscopic beam, to resolve volume averaged but localised characteristics from statistically representative sample volumes. We then analyse the variation of mineralogy, mineral orientation, porosity and pore orientation, including pores from 1-150 nm size.

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Validating the use of gas slippage measurements for pore structure characterisation by comparison with predictions from bundle of capillary tubes models

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Characterising pore structure geometry is fundamental to understanding and predicting many aspects of porous media behaviour. Tight rocks typically have sub-nanometer to micrometre scale pore size distributions, rendering characterisation of their pore structures challenging in comparison to higher permeability rocks with larger pores. Not all techniques developed and refined for characterisation of the larger pores found in more permeable rocks are applicable to tight rocks, and many commonly used techniques when applied to tight rocks often lead to incorrect characterisations. Here we investigate the validity of using gas slippage measurements as a pore structure characterisation technique by comparing pore sizes calculated from gas slippage measurements with those predicted by bundle of capillary tubes models. A large data set of gas slippage measurements was generated by combining our gas slippage measurements for a suite of tight rocks (48 measurements of rocks at different stress states with permeabilities as low as 10-22 m2) with published gas slippage data sets for higher permeability reservoir rocks (permeabilities as high as 10-11 m2). Estimates of pore size were calculated for all of the gas slippage measurements in the compiled data set using both the cylindrical and slot-shaped pore geometry models. The trend of the compiled data set in pore size - slip corrected permeability space was compared to the trend predicted by a simple bundle of capillary tubes model informed by porosity data from the data set and a theoretical tortuosity-porosity relationship from the literature. Pore size calculated using the slot-shaped pore geometry resulted in good agreement with the trend predicted by the bundle of capillary tubes model. This result quantitatively validates using gas slippage measurements as a pore structure characterisation technique. Pore structure characterisation using gas slippage measurements is especially well suited for analysing the pore structures of tight rocks due to the highly stress sensitive nature of these rocks; gas slippage measurements can easily be made on samples at their stress state of interest, whereas many commonly applied techniques cannot (e.g. mercury intrusion porosimetry, scanning electron microscopy, and CO2 and N2 adsorption). Additionally, scale of resolution is not a limitation for gas slippage measurements, but is a limitation for analyzing tight rocks using many techniques commonly used. Gas slippage measurements however result in a calculation of average pore size, whereas other techniques can provide insight into the distribution of different pore sizes within a rock. With the tools currently available, adequate characterisation of pore structure in tight rocks thus relies on the combined use of many tools with due consideration to their strengths and limitations.

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Water vapour sorption by mudrocks

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High-resolution water sorption isotherms were measured on 13 representative mudrock samples in order to assess the mechanisms of water vapour sorption and their relation to the pore structure of mudrocks. The measurements were performed at 303 K on a gravimetric, dynamic vapour sorption device. Experimental data were interpreted by traditional physisorption models for which the validity was evaluated by relating model parameters to those obtained from nitrogen physisorption measurements. No direct relations with the pore structure were observed, except for Gurvich total pore volumes and corresponding porosity data. Specific surface areas from Brunauer-Emmett-Teller theory are ambiguous and do not relate to nitrogen data suggesting that water molecules do not adsorb as (multi-) layers covering pore walls. The Volume Filling Theory (Dubinin-Astakhov-Equation) fits the water sorption data well but no relation to nitrogen data was observed in the studied sample set. A lower affinity of water for micropores was evident from the higher filling pressures of N2-based micropore volumes. Barret-Joyner-Hallenda theory combined with N2 physisorption measurements on moist mudrocks revealed that capillary condensation prevails close to saturation but not below about 0.94 p/p0. A distinct low-pressure hysteresis was observed from hysteresis scanning which was attributed to surface chemistry since capillary condensation occurs only at very high relative pressures. Analysis of mineralogical composition, TOC and organic maturity in relation to water sorption revealed only a weak correlation with the total clay content. In contrast, CEC strongly correlates with water uptake, which evidences a surface chemistry controlled sorption mechanism. Tests of the influence of the exchangeable cation were inconclusive because pore system alteration due to cation-exchange likely superimposed the effect. To further assess the sorption mechanisms of water, nitrogen physisorption isotherms were measured on moisture-equilibrated mudrocks (11, 52, 75, 94 %RH at 298 K). Micropore analysis and cumulative pore size distributions denote that water rather blocks pore throats than fills pore volume at lower relative humidities. Over the entire humidity range, no direct relation between water sorption and pore size was observed. These findings imply that water adsorption does not sequentially fill pores with increasing radii in mudrocks as relative humidity increases, as would be expected from water sorption by capillary condensation. This conclusion has important implications for the interpretation and measurement of geomechanical and petrophysical properties of mudrocks. Capillary pressures, particularly at low water saturations, are often calculated from water saturation using a concept based on the Kelvin equation for capillary condensation. Since water sorption in mudrocks seems to be controlled by surface chemistry rather than pore size, this approach is questionable. The observations reported here suggest that the water distribution in mudrock pore systems resulting from vapour equilibration differs from that obtained by fluid displacement, i.e. capillary drainage or imbibition. A further consequence is that water vapour equilibration is a convenient but not necessarily representative method to obtain partially water saturated mudrock samples for laboratory measurement of saturation-dependent geomechanical or petrophysical properties.

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X-ray micro CT for structural and compositional analysis of cores at different scales (dm -> µm)

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Introduction

Recently non-destructive investigations using X-ray Computed Tomography (CT) of geomaterial became more and more important. For geomechanical investigations it is essential to get information about the mineral composition, its spatial distribution, pores, and fractures to increase the understanding of deformation processes. In this study a clay core of 100 mm diameter was sub-sampled down to ~30 mm and finally 3 mm diameter and analysed by X-ray CT and various conventional petrophysical analysis.

Material and Mechanical Testing

The specimen “file 13001” (drilling BLT-A6, diameter 100 mm, length 180 mm) was derived from the Underground Rock Laboratory Mont Terri (Switzerland) from the sandy facies of the Opalinus Clay (Kaufhold et al., 2013). The claystone was investigated under undrained condition by triaxial strength tests until a failure was developed. After the mechanical testing the core was embedded in resin to stabilize the specimen.

X-ray CT results for different scales

The 100 mm Opalinus Clay sample was first scanned with the speed|scan CT 64 (GE Ahrensburg, Germany). The scan was recorded within 13 seconds at a spatial resolution of approx. 0.3 mm. The reconstruction was performed automatically (Ambos et al., 2014), therefore the 3D data could be evaluated after 30 seconds. The CT results show good contrast resolution due to its high power (up to 72 kW), layering within the core can be nicely detected (see figure 1). Cracks and pores are spatially resolved down to 0.5 mm.

Figure 1 Virtual sliced 3D view of the speed|scan CT result shows inner structure (layering, cracks).

Secondly, a CT scan of the same sample was recorded with the v|tome|x L300 system (GE Wunstorf, Germany) with a scan time of 145 min and a spatial resolution of approx. 60 µm. Fractures are much better resolved (down to ~60 µm)and the delicate network can be nicely visualized (see figure 2).

Figure 2 Transparent 3D view of the L300 CT data. Cracks are segmented (red colour).

For the 30mm and 3mm samples a nanotom m system (GE Wunstorf, Germany) enabled for 120 min scans a resolution of 18 µm and 3 µm respectively. Due to this high resolution one can detect tiny fractures down to approx. 3 µm (see figure 3).

Figure 3 Virtual slice of the nanotom m CT data (Cracks width ~ 3.5 µm).

Conclusions and Outlook

The fast analysis with X-ray CT based on medical scanners (speed|scan CT 64) is suitable to give an overview of large core. However microfocus (v|tome|x L300) and nanofocus tubes (nanotom m) can provide much more detailed images necessary for special high resolution core analysis. The overall aim of the investigation of the Opalinus Clay is to understand the rock deformation processes upon mechanical stresses. This behaviour is largely governed by microstructure thus CT is a key method. Additionally, chemical and mineralogical methods are used to identify homogeneous areas which can be considered representative of the entire rock. Hence, the CT information gathered from a small volume can be used to understand the mechanical processes of the entire rock.

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A molecular theory for optimal blue energy extraction

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Electrical double layer expansion (CDLE) has been proposed as a promising alternative to reverse electrodialysis (RED) and pressure retarded osmosis (PRO) processes for extracting osmotic power generated by the salinity difference between freshwater and seawater. The performance of the CDLE process is sensitive to the configuration of porous electrodes and operation parameters for ion extraction and release cycles. In this work, we use a classical density functional theory (CDFT) to examine how the electrode pore size and charging/discharging potentials influence the thermodynamic efficiency of the CDLE cycle. The existence of an optimal charging potential that maximizes the energy output for a given pore configuration is predicted, which varies substantially with the pore size, especially when it is smaller than 2 nm. The thermodynamic efficiency is maximized when the electrode has a pore size about twice the ion diameter.

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Designing and Testing Universal Ion-Exchange Membranes based on Carbon Nanotubes

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Ion-exchange membrane technology is a rapidly developing field which finds applications in waste water treatment including separation of complex mixtures of chemical compounds, extracting energy from concentrates, and most important: The production of drinking water from salt water through desalination. Electrochemical desalination occurs through electrodialysis (see figure)[1]. A voltage is applied across salty water, separating the cations from the anions. An ion-selective membrane prohibits the diffusion of ions with an opposite charge. As a result, desalinated water is produced.

Currently, membranes are made specifically as cation exchange membranes (CEM) or anion exchange membranes (AEM). A long standing aim is to produce an electronically controllable universal ion-exchange membrane which can be switched from CEM to AEM. Carbon nanotube (CNT)-based membranes are identified as high potential candidates for the realization of said controllable membranes, as CNT have unique and tunable physicochemical properties, such as electrical conductivity and well-defined dimensions [2, 3].

We present newly designed configurations for an optimal CNT-based membrane. We have used a Focused Ion Beam-Scanning Electron Microscope (FIB-SEM) for rapid prototyping. In addition, the FIB-SEM is used to determine the exact 3D dimensions of the membrane and exclude the presence of meso porosity within the membranes. The advantage of CNT-based membranes is their well-defined porosity, predominantly formed by the straight tubes. As a result, we are able to correlate the electrochemical characteristics with the physical appearance of the CNT-based membranes (e.g. porosity, membrane thickness, etc).

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DYNAMIC THEORY OF ION ADSORPTION IN POROUS CARBON ELECTRODES

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Desalination technologies like capacitive deionization (CDI) use porous carbon electrodes to desalinate water by storing ions in electrical double layers (EDLs). In modeling the transport of ions in CDI, electrosorption process can be described by the occurrence of two processes [1]: (i) transport of ions through the pore space between carbon particles, macropores, and (ii) ion adsorption in the internal pores of the carbon particles, micropores, where EDLs are formed. A simplified way to describe the dynamics of ion electrosorption into the porous electrodes is to neglect salt concentration gradients and potential gradients in the macropores. With this approach we assume that the transport from macropores-to-micropores and vice versa is rate-limiting. In this work EDLs are described using the amphoteric Donnan (amph-D) model which considers chemical information of the surface of carbon electrodes [2]. Theoretical results are compared with experimental data obtained using wire-shaped electrodes coated with ion exchange membranes (IEMs) and without IEMs. The presented dynamic theory can be can be applied not only to wire electrodes, but also to conventional CDI with flat porous carbon electrodes.

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How surface conduction and random pore coupling can affect electrokinetic transport in porous media

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Electrokinetic transport in porous media involves complex dynamics that can be utilized in various technological applications including supercapacitors for energy storage [1], deionization and purification systems [2], and lab-on-a-chip devices [3]. Due to high surface to volume ratio in these systems, surface conduction, through electric double layers (EDLs), can play an important role in charge transport that can lead to nonlinear dynamics such as deionization shocks [4, 5]. This nonlinear behavior activates a mechanism for overlimiting current in these structures [6], which allows higher rates of ion transfer beyond diffusion limitation. These effects are well understood for a single pore, however coupling of nonlinear modes of electrokinetic transport in networks of many pores is yet to be understood. Additionally, when the pore size varies randomly in space electrokinetic effects can induce internal flows, that can couple with nonlinear modes of transport in an unintuitive way.

We have developed an efficient model that can accurately captures the aforementioned nonlinearities inside porous media. The computational cost of our model is multiple orders of magnitudes less than that of brute force calculations using direct numerical simulations. We model a porous medium as a network of one-dimensional pores that are coupled at the pore intersections. A one-dimensional transport equation is derived for each pore that describes the cross-sectional averaged concentration as a function of time and pore longitudinal coordinate. While similar approaches have been attempted in the past, our model offers unique advantages that make it highly desirable for numerical simulations. Advantages of our model includes: (1) There is no limitation on the local EDL thickness, (2) The model is discretely conservative with zero numerical leakage of ions, (3) The model coefficients are bounded and do not involve singularities in the limit of thick EDLs, (4) The model is well balanced; it recovers the equilibrium solution exactly in the absence of external driving forces, (5) The model naturally allows analysis of transport in a massive network of many pores and can handle discrete jumps in pore sizes or multi-pore intersections. The simulation approach presented by the developed model bridges the gap between traditional homogenization methods, which fail to capture the pore-scale nonlinearities, and expensive direct numerical simulations (DNS), which have to resolve complex geometries in multi-dimensions. Using this model, we demonstrate simulations of massive networks of pores, and discuss the impact of couplings between surface conduction and pores' random connectivity on macroscopic behavior and transport rates in porous media.

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Nanostructured pseudocapacitive electrodes for water purification and environmental remediation

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The development of functional porous materials is crucial for solving water scarcity and environmental challenges in the 21st century. Capacitive and pseudocapacitive deionization are promising technologies for water treatment, in which major focus has been devoted to creating high surface area, conductive electrodes [1]. In particular, an emerging direction has been the design of redox-active electrodes through combination of the structural advantages of porous architectures with accessible Faradaic units [2]. Through the tuning of a specific Faradaic reaction, we are able to specifically bind certain ions of interest with significant uptake capacities, and also increase electrochemical performance. Here, we report advances in the development of chemically-selective interfaces based on both organic and organometallic species to target a variety of specific ionic contaminants for separation, enable redox-mediated pollutant transformation, and more recently, effect bulk deionization. First, with these redox-polymers supported on nanoporous electrodes, we investigated a series of metallocene-functionalized surfaces to adsorb and release organic ions with high separation factors (>300) and uptake capacities (>200 mg/g), targeting functional groups such as carboxylates, sulfonates, and phosphonates, as well as heavy metals and relevant cations [3]. Second, we present porous hierarchical electrodes with hemin-based metal complexes for the selective binding and electrocatalytic degradation of neutral contaminants, with high turnover numbers (>700) and low overpotentials. Finally, we present recent results obtained with an asymmetric electrode configuration (dual redox-design) for deionization at low to dilute concentrations (<10 mM ionic strength) and discuss their energy performance relative to that of existing systems, both in flow and in batch. For all these cases, we discuss both the materials characterization and the in-depth mechanism for interfacial adsorption. In general, we are expanding the library of chemically-functionalized porous electrodes for applications in water treatment, product purification and environmental electrocatalysis, and, through both pore architecture design and immobilization chemistries, we can achieve robust interfaces for practical implementation in the near future.

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Porous-media flow, ionic transport, and dispersion in Na-ion desalination devices and redox flow batteries

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Worldwide installed desalination capacity has been established primarily by mechanical and thermal approaches, but alternative technologies exist that use electric potential as a driving force to deionize water. We predicted recently that a Na-ion battery using low-cost, high-capacity intercalation host compounds (IHCs) can desalinate seawater level salt concentrations [1]. Furthermore, a minimal number of membranes can be used to desalinate with low energy consumption if a flow-through electrode configuration is employed. The electrodes within such systems are heterogeneous composite, porous materials containing solid IHCs to store Na ions, carbon black to conduct electrons, and saline water electrolyte from which ions are extracted to produce desalinated water. In this context, tortuosity impedes species transport and the fine scale of their porosity induces dispersion. In this work, we explore the effects of electrode microstructure and two-dimensional superficial flow patterns on the energy consumed during water desalination. Energy storage technology for the electric grid is becoming increasingly important to promote sustainability for electricity generation, including to buffer the intermittent power supply from renewable energy sources (e.g., wind and solar). The massive amount of energy generated in these applications requires energy storage architectures that are scalable. One such device is the redox flow battery, which stores electrochemical energy within redox-active molecules dissolved in electrolytes. The reactors of such devices contain porous current collectors that are used to transfer electrons between the external circuit and redox-active molecules. As redox-active electrolyte is flowed through these electrodes there is a competition between transverse ionic conduction, the deleterious crossover of active species, dispersion, and pumping pressure. Here, we explore the interplay between these effects, thereby identifying strategies to enhance device performance through cell and materials engineering.

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Water desalination using Capacitive Electrodes: from Carbon Nanotube Membranes to Activated Carbon Suspensions

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Carbon can desalinate water in several ways. In the first approach, a carbon material with thin pores such as carbon nanotubes (CNTs), with pores of a few nm in diameter, is used to selectively separate water from ions [1,2]. CNTs acquire a surface charge by interaction with water (charging negatively), but can also be electrically addressed so the charge can be changed at will. In the second approach, porous carbon electrodes are cyclically charged and discharged, resulting in the periodic adsorption and desorption of ions [3,4]. In this process, called capacitive deionization, one electrode preferentially adsorbs cations, and the other anions. Data for carbon charging and desalination help to validate models of the structure of the electrical double layer in the water and in the carbon [5]. For micropores in activated carbon, the Donnan approach (effectively smearing out the potential) is shown to describe data accurately [5]. We describe experimental approaches for capacitive water desalination using film electrodes as well as electrodes in the form of a slurry and fluidized bed, where carbon beads are pumped around a circuit, charging in one part of the system, and discharging elsewhere [6]. We show how upon contact, oppositely charged beads release salt.

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Creation of In-Situ EOR Foams by the Injection of Dispersed Foamer in Gas, and its Application in a Piedemonte Oil Field (Colombia).

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This work presents the conceptual development, the experimental evaluation and a field pilot application for a new technique to create in-situ EOR foams based on the injection of the foaming agent dispersed in the hydrocarbon gas stream. This new technique aims at: 1) simplifying and reducing costs for the deployment of EOR foams in gas injection based projects, and 2) overcoming the disadvantage of limited reservoir volume of influence obtained during most of the conventional Surfactant Alternating Gas (SAG) implementations.

The concept behind this new technique is the transfer of chemical foamer from the gas dispersed phase into the connate or residual waters present in the hydrocarbon reservoirs under exploitation, due mainly to the big chemical potential derived from the contrast in chemical foamer concentration between the dispersed phase and the in-situ water. A systematic experimental work is presented for the first time, as far as the authors are aware of, investigating the effect of the dispersed chemical (surfactant) concentration on the ability to create blocking foams with hydrocarbon gas at high pressure and temperature; and using representative consolidated porous medium and fluids coming from the Piedemonte fields.

Results herein confirm that in fact it is possible to create blocking foam by injecting the foaming chemical dispersed in the hydrocarbon gas stream into a consolidated sandstone core at residual oil and water conditions, after being submitted to a gas flooding displacement. This condition is obtained as far as the gas velocity is above a minimum threshold, and the concentration of the active chemical is above certain limit (138 ppm for this case). Successful experiments with foams created by this method showed much longer stability periods when compared with results from foams created by the SAG technique at much higher chemical concentration (2,000 ppm). On the other hand, dynamic adsorption tests showed similar equilibrium adsorption values when the foaming chemical is injected dispersed in the gas as compared with the liquid batch case, for comparable chemical concentrations.

Application of this innovative foams technique was implemented in a field pilot. About 600 Bbls of foaming solution at a rate of 1 Bbl/MM scf were injected in the hydrocarbon gas stream in one gas injector of a Piedemonte field for a period of two(2) months. Gas injectivity in the well was impaired after two weeks of injection, and the oil production well influenced by this injector changed its performance showing incremental oil production and flattening of the gas oil ratio (GOR) shortly after the dispersed chemical injection period. These results confirm that the new technique can be implemented at the field scale, and incremental production can be obtained from it in reservoirs operated under hydrocarbon gas injection. The technique could also be extended to other non condensable gases at field operating conditions such us CO2, Nitrogen, Air, and Flue gas.

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Evaluation of water drying due to gas injection in foam-based well conformance operations and its effects in foam generation and stability.

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Foam generation in porous media strongly depends on the existence of a mobile aqueous phase. The snap-off generation mechanism is triggered by the presence of mobile water that allows the lamella genesis in the pore throat. A low water saturation generates high water capillary pressures, increasing the lamellae coalescence rate and then foam stability is reduced. When the water saturation tents to an irreducible value, the foam generation tents to cero. Just as the water evaporates, other components increase their concentration, such as salts and surfactants that strongly affect the foam behavior. By studying all the coupled phenomena associated to the gas injection for foaming, the effects of dry gas injection over the foam generation and stability can be done. Therefore, the objective of this study is to evaluate the impact of reservoir water drying in the porous media on the foam generation and stability through an advanced phenomenological model. The model is based on a multicomponent/multiphase flow model (oil, gas & water) with water evaporation/condensation, coupled to a lamellae (foam) population balance equation. We simulated the injection of dry gas into a reservoir having high vertical heterogeneities and permeability with anisotropy in order to quantify the reduction in the foam generation and stability. We found that during dry gas injection two counteracting phenomena occurs. The gas phase displaces the liquids (oil and water) into the formation. The unsaturated gas creates a water evaporation front that is propagated as injection proceeds, reducing the water saturation, even below irreducible values. This saturation gradient generates a counterflow water flow due to capillary effects, that in turns helps to avoid a complete drying.

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Evolution of the bubble size distribution in a foam flowing through a 2D porous medium

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Foams have been used for decades as displacing fluids for EOR and aquifer remediation, and more recently as carriers of chemical amendments for the remediation of the vadose zone. Apart from various interesting physico-chemical and biochemical properties, foams are better injection fluids due to their low sensitivity to gravity and their peculiar rheology: for foams with bubbles on the order of at least the typical pore size, viscous dissipation arises mostly from the contact zones between the soap films and the walls.

In most experimental studies no local information of the foam structure is possible, and only global quantities such as the effective viscosity can be measured. In a recent study, we investigated the flow of an initially monodisperse foam through a transparent two-dimensional porous medium consisting of circular obstacles positioned randomly in a horizontal transparent Hele-Shaw cell [1]. The flow exhibits a complex phenomenology, which can be characterized quantitatively from optical measurements of the bubble dynamics. In addition to preferential flow path and local flow intermittency, we observed selection of the bubble size distribution by the medium, through lamella division-triggered bubble fragmentation. Lamella division is one of the known mechanisms of lamella creation; it occurs when a bubble is pinched against an obstacle. In our model two-dimensional porous medium, lamella division is by far the dominant mechanism of lamella creation/destruction, which results in an irreversible evolution of the bubble size distribution as the bubble travels along the porous medium.

In this study we focus on the understanding and modeling of this evolution of the probability density function (PDF) for bubbles size. We measure and characterize this evolution as a function of the experimental parameters. The observation of the lamella division around specific obstacles provides the statistics of the bubble fragmentation rate and of the fragment size distributions. These two ingredients and the measurement of the initial bubble size distribution allow modeling the bubble size PDF evolution process numerically, based on a fragmentation equation, with excellent agreement. The modeling also predicts a nearly-universal scaling of all PDFs as a function of the bubble area normalized by the initial mean bubble area. All the measured PDFs, obtained with different mean flow velocities, initial bubble sizes and foam qualities, collapse on a master distribution which is only dependent on the geometry of the medium.

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Experimental Investigation of the Effect of Oil on Steady-state Foam Flow in Porous Media

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Foam flow in porous media without oil shows two regimes, depending on foam quality (gas fractional flow) (Alvarez et al., 2001). Complexity and limited data on foam-oil interactions in porous media greatly restrict understanding of foam in contact with oil (Farajzadeh et al., 2012). This knowledge gap hinders reliable design and performance prediction for foam enhanced oil recovery (EOR). We report steady-state corefloods to investigate the effect of oil on foam through its effect on the two foam-flow regimes. Then, for the first time, using a method similar to that of Cheng et al. (2000), we fit the widely used STARS foam model parameters to the experimental data for local-equilibrium (LE) foam flow in presence of oil. This research provides a practical approach and initial data for simulating foam EOR in the presence of oil.

To ensure steady state, foam is co-injected with oil at fixed oil superficial velocity (Uo) and at a fixed ratio of oil to water superficial velocity (Uw), respectively, in a Bentheimer sandstone. Model oils used here consist of two components: hexadecane, which is benign to foam stability, and oleic acid, which can destroy foam completely. Varying the proportion of oleic acid in the model oil allows one to examine the effect of oil composition on steady-state foam behaviour. Experimental results show that the presence of oil impacts both high- and low-quality regimes. The high-quality regime, dominated by foam stability, is more vulnerable to oil, especially oleic acid, which destabilizes foam. The shift in the high-quality regime demonstrates that oil weakens foam by increasing the limiting water saturation for foam stability. Furthermore, this regime is strongly shear-thinning in the presence of oil. Pressure gradient in the low-quality regime, in some cases, decreases with increasing Uw at constant gas superficial velocity (Ug), whether or not oil is present. This may reflect an effect of oil, if oil is present (Tang et al., 2016), or the easier flow of foam bubbles under wetter conditions (Kim et al., 2005). Increasing the oleic acid concentration shifts the low-quality regime to lower foam qualities, indicating greater difficulty in stabilizing foam. Our data indicate that oil composition plays a more significant role than oil saturation in foam stability.

Our parameter-fitting method assumes an abrupt transition between the two regimes. Shear-thinning behaviour in the low-quality regime is included. The fitted parameters indicate an increase in limiting water saturation in the presence of oil, especially with oleic acid, and easier flow of bubbles in the low-quality regime in the presence of oil. None of current foam simulation models can represent the decrease in pressure gradient with increasing Uw at fixed Ug in the low-quality regime without oil.

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Experimental Study on CO2 Foam flow Characteristics in Porous Media

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In homogeneous porous media prepared with the sand packing method, the simulative experiments were carried out for CO2 foam flooding process and the CO2 foam flow characteristics in porous media were studied with the help of CT technology. CO2 foam flooding experiments were carried out under different packing sand sizes, different surfactant concentrations and different gas-liquid ratios. CT technology was employed to visualize the displacement process and to obtain the water saturation data along the sample, and in the same time, the pressure distribution in the sample in the foam seepage process was also measured. Experimental results show: CO2 foam flooding has higher pressure drop and lower water saturation entrance effect in the porous media with lower average grain sizes; when surfactant concentrations are higher than CMC (Critical Micelle Concentration), the generated foam is stable with no obvious difference for the foam displacement efficiency, and the water saturation entrance effect gradually decreases with increasing surfactant concentrations; improved gas-liquid ratio could increase the foam seepage pressure drop, however has little effect on residue water saturation after foam displacement.

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Foam Coarsening: Behaviour and Consequences in a Model Porous Medium

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Gas injection was introduced to the petroleum industry in the early 1950s. Nevertheless, the process efficiency is impacted by the low density and viscosity of the gas, which decrease sweep efficiency. Foam for Enhanced Oil Recovery (EOR) can overcome the downside of the viscous fingering by increasing the apparent viscosity of the gas. Importantly, the structure of the foam evolves with time due to gas diffusion between bubbles (coarsening). In a bulk foam, the coarsening behaviour is well defined, but there is a lack of understanding of coarsening behaviour in confined geometries, especially in porous media. Nonnekes et al [1] predicted numerically and analytically that coarsening will cause the foam lamellae to move to low energy configurations in the pore throats, resulting in greater capillary resistance when trying to restart flow. This study describes the foam coarsening in porous media and the implications for foam propagation. Foam coarsening experiments have been conducted in both a micromodel and in core material. The micromodel is etched with an irregular hexagonal pattern, with a Gaussian distribution of pore diameters. Foam was generated by coinjecting surfactant solution and nitrogen gas into the micromodel through a 10 µm frit. Once steady state flow had been achieved, the flow was stopped and the chip sealed off. The coarsening behaviour of the foam was recorded using time-lapse photography. The core material coarsening experiments were carried out using a Bentheimer Sandstone core. Foam was produced by coinjecting surfactant solution and nitrogen at the base of the core. Once a steady state flow was achieved, the flow was stopped and the core sealed off. When flow restarted, the additional driving pressure required to reinitiate flow was measured, and this could be attributed to the stable configuration of the coarsened foam. The microfluidic results found that the bubbles coarsened rapidly ($t < 10$ minutes) to the size of the pores. At the completion of coarsening the majority of the lamellae were located in the pore throats with minimum length. Because of the effect of the walls, the behaviour did not conform to the unconstricted coarsening growth laws. Furthermore, results on coreflood showed that coarsening is a rapid process, in agreement with microfluidic results. An increase in the additional pressure required to re-initiate flow was observed for the first 1 – 5 minutes of flow stoppages, while the pressure peaks did not increase for durations above 5 min. The implications of this behaviour for the field scale are also discussed.

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Foam generation, apparent viscosity and flow in fractures

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Foam for gas mobility control in porous media is substantially covered in literature, mainly in the petroleum-related literature with focus in porous rocks. A less focused research area is foam generation in fractured systems, with both experimental and modeling (Kovscek et al., 1995, Pancharoen et al., 2012). A recent investigation of foam generation in a rough-walled fractured system demonstrated foam generation during co-injection of surfactant solution and gas to effectively reduce gas mobility in fractures (Fernø et al., 2016). The current experimental work further investigates foam flow in fractured systems of different size and geometry, with the overall objective to evaluate the impact of trapped gas and system design.

Systems A and B constitute fractured marble cores with diameters of two and four inches with rough-walled fractures. The total volumetric rate was kept constant during all co-injections, and the gas fractional flow was varied in pre-defined fractions. Measurement of differential pressure was corroborated by visual inspection of strong, fine-textured foam at the outlet. Foam rheology was evaluated using different flow rates in each system, and apparent viscosity of foam was found to decrease at increased flow rates, hence, suggesting a shear-thinning foam behavior. Foam flow did not seem dependent on system size, although an exhaustive experimental sensitivity was not performed: the strongest gas fraction was observed at high gas fractional flow, and pressure response was similar for both systems.

Positron emission tomography (PET) imaging was successfully applied to visualize liquid saturation and distribution during co-injection for foam generation in fractured systems. The PET imaging technique is frequently used in hospitals to diagnose malignant cancer tumors. PET application in geo-sciences was recently demonstrated in quantitative water saturation measurements (Fernø et al., 2015a), CO2 storage (Fernø et al., 2015b) and other industrial applications such as EOR measures using polymer gels in fractured systems (Brattekås et al., 2016). During co-injection for foam generation and flow, PET provided imaging of local surfactant concentrations within the fracture network, and access to variations in the saturation contributed to understanding observed differences in measured differential pressures. Our results suggest a substantial saturation of trapped gas, presumably due to a high gas saturation prior to decreasing the gas fraction during co-injection.

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Gravitational effects on foam flow in 3D printed heterogeneous porous media in the presence of oil

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Foam is often used in improved oil recovery processes to displace oil from underground reservoirs as well as in soil remediation practices. Foam flow in porous media is indeed a complex phenomenon and the dynamics of the phase distribution during oil displacement is influenced by a variety of parameters such as foam quality, heterogeneity, and type of oil [1-6]. In recent years, there has been a rising interest in experimental investigation of foam flow in porous media with sophisticated imaging tools to delineate the governing mechanisms controlling this process. However, the majority of these experiments were conducted under minor impact of gravity (horizontal flow). The specific objective of this work was to investigate the effect of flow direction relative to gravity on foam flow behaviour. To elucidate this effect, a compressive series of experiments have been performed in porous media (110mm by 50mm) manufactured by 3D printing technology in horizontal and perpendicular direction with respect to gravity. The pore network was created from a Voronoi diagram. The pore throat size was randomly distributed in the network using a normal distribution of sizes ranging from 0.8 to 1mm. The depth of the porous medium was 0.5 mm. Foam was generated in situ following simultaneous injection of gas and surfactant with four flow rates of 5, 10, 20 and 40 ml/h in each horizontal and vertical direction. A computer-controlled monochromic camera was fixed in front of the model to acquire images of the displacement process at regular time intervals. The recorded images were analysed using in-house codes developed in MATLAB. The obtained pore-scale information enabled us to accurately investigate foam generation, coalescence, and propagation as influenced by gravity and the injection rate. One of the key impacts of gravity was related to the phase separation (due to density difference) which remarkably influenced the foam propagation in porous media and its sweep efficiency. Also, the obtained results indicated that phase separation decreased as the flow rate increased. The observed behaviours highlight the significant impact of gravity on foam performance echoing the necessity to include gravitational effect when investigating oil displacement by foam in porous media.

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Mechanism of nanoparticle-stabilized foam generation in the presence of a brine

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Surfactant-stabilized foam is employed to enhance oil recovery and remediate contaminated soils because of the advantages in improving mobility control and increasing sweep efficiency. One of the major drawbacks is foam destabilization during transport due to the adsorption of the surfactant onto the porous media surface (Lv et al., 2015). Nanoparticles have been observed to improve the foam stability because they adsorb at the gas-liquid interface create an armor, which prevents foam destruction (Binks, 2002; Kam and Rossen, 1999). The larger the nanoparticle concentration the high is the foam stability. However, nanoparticles might create a resistance to foam generation particularly at large concentrations increasing the threshold of pressure drop to initiate bubble formation. Current mechanistic foam transport models do not account for the effect of nanoparticle on the kinetics of foam generation and it is the aim of this work to understand the generation mechanism of a nanoparticle-stabilized foam in order to formulate a constitutive equation for the rate of generation, which accounts for the presence of the nanoparticles and their concentration. Here, we present microfluidic experiments to observe the foam generation at the pore scale. Initially, we saturated the porous medium chip (as shown in Figure 1.a.) with a surfactant solution containing a known concentration of sodium chlorite (NaCl), namely 0.5 wt.%. Then we injected air with a syringe pump at constant flow rate (between 100~400 uL/min). Continuously, the experiments were monitored with a high-speed camera to capture the evolution of the foam texture with pressure drop. Preliminary results for a foam stabilized with a surfactant (SDS at 0.5 wt.%) are shown in Figure 1.b. Here, it is possible to see that foam generation occurs suddenly when a certain value of pressure drop (dP, psi) is reached at constant gas injection rate. Our hypothesis is that such a behavior, previously observed for a surfactant-stabilized foam (Gauglitz et al., 2002) is still occurring for a nanoparticle-stabilized foam and experimental activity to verify it is ongoing. We expect that the threshold value of dP (dPmin) changes with nanoparticle concentration as observed in our earlier work for CO2-foam stabilized with nanoparticles and surfactant (Prigiobbe et al., 2016) and that at same conditions dPmin for nanoparticle-stabilized foam is larger than for a surfactant-stabilized foam. It is the aim of this study to gain an insight into the generation mechanism of a foam solely stabilized with nanoparticles through a series of systematic experiments monitored with online sensors.

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Modelling sweep efficiency improvement by in-situ foam generation using foamer droplets disperse in the gas stream.

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Foam generation and transport in porous media is a proven method to improve the sweep efficiency of a Flooding fluid in EOR process and the effectiveness of a treatment fluid in well intervention procedures. The foam in the porous media is often generated using SAG (Surfactant alternating gas) or Co-injection. Although these operations result in a good incremental production, the profit losses are high due to surfactant retention and lack of water injection facilities in the target fields. One way of reducing the costs of foam generation operations is by injecting the foamer/surfactant solution disperse throughout the gas phase in a process called “Disperse Foam”. Core flooding experimental results have proven that disperse foam techniques reduce the foamer/surfactant retention and increases cumulative oil production. This increase means that not only is the foam being generated but also it is blocking the high mobility channels and enhancing the sweep efficiency. Additionally, the upscaling from laboratory to field injecting conditions is very simple and reduces significantly operational costs of the process. Because few laboratory core flooding tests and field pilots have been implemented using the disperse foam technique, there is a high level of uncertainty associated with the process. Moreover, the models reported in the literature do not account for all the associated phenomena, including the surfactant transfer between the gas and liquid phases, and the lamellae stability at low water saturations. For this reason, the development of a mechanistic disperse foam model is the key to understand the phenomena related to disperse foam field operation. In this work, we use a previously developed mathematical model to simulate different heterogeneous well scale scenarios to predict the oil sweep efficiency and compare the disperse surfactant method, SAG and co-injection. The mathematical model accounts for the non-equilibrium mass transfer of foamer between the gas and liquid phases. In addition, the dynamic reversible and irreversible adsorption of surfactant on the rock surface is accounted for using a first order kinetic model. The foam generation, coalescence and transport is modeled using a mechanistic population balance model. Simulation results show that the co-injection technique allows for a deeper foam creation than the SAG mode. However, higher foam stability is achieved in the later.

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Monitoring the position of a foam front in a 3D pilot

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Injection of foam is an enhanced oil recovery (EOR) method used in petroleum engineering applications as it increases the volumetric sweep of the oil reservoir compared to conventional gas injection processes by lowering the mobility of the injected gas. In this study we investigate whether a foam injection process is also suitable for groundwater applications which means unconsolidated porous media resulting in higher permeability, considerably lower operating pressures and additional environmental constraints on the substances used during the process. This study focuses on the use of foam for confining a contaminant source zone in a porous medium. Thus, the ability of foam to block flow of groundwater is of importance. (i.e. its mobility needs to be significantly lower than that of water). In addition, the volume of the porous medium where the foam has swept needs to be determined. To this end, foam is injected into a 3D pilot with dimensions of approximately 1 x 1 x 1 meter. This size was chosen as this experiment serves as a pilot study for a real field test, thus experimental techniques used here need to be feasible on a field scale as well. As such, methods for determining saturations of fluids that can be used on a lab scale such as the use of CT imaging are not applicable here. Two vertical are placed in opposite corners of the pilot that serve as injection and production well respectively with radial flow of foam between the two resulting in a quarter give-spot pattern. Several different measurement methods are considered in this experiment to monitor the location of the foam front during the injection process. Pressure measurements are performed to determine the pressure drop over various sections of the pilot which provide a measure for the mobility reduction caused by the foam. A porous medium fully saturated with water has different acoustic (wave velocity) and resistive properties thus acoustic imaging and electrical resistivity tomography are employed in this experiment to monitor the location of the foam front during the injection process. In addition, optical probes are used locally to determine fluid properties based on color. By dying the liquid that is initially in place, the optical response differs once the undyed foam has swept. Results from these experiments will be used to identify foam model parameters and determine whether the water relative permeability is affected along with that for gas.

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Multi-Scale Experimental Study to Define the Effectiveness of Foam to Reduce Global Mobility in an Aquifer

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Foams are widely used in petroleum industry for enhanced oil recovery (EOR), and a lot of fundamental work has been done on foam in porous medium. Foam is defined as a dispersion of gas in liquid in which the gas is made discontinuous (i.e. trapped in separate bubbles) by thin liquid films called lamellae. These lamellae are stabilized by surfactants. The trapping of gas in bubbles means that its ability to flow inside a porous medium is impaired thus reducing its mobility. As such, injected foams can provide a more stable displacement front as free gas flow tends to suffer from viscous fingering, channeling through high-permeability layers and gravity override thereby limiting the volumetric sweep of the reservoir or aquifer. Commonly, the effectiveness of foam is quantified by its ability to reduce the overall mobility. Strong foams, characterized by very fine bubbles and stable lamellae provide the best reduction of mobility, whereas weak foams leads to low reduction mobility due to instabilities of lamellae. During an injection process in the lab or field, the foam's strength can be determined through pressure measurements. Larger pressure gradients imply a stronger foam able to block fluid displacement in porous medium

We first investigate a commercial biodegradable surfactant and assess its ability to create strong foam at reasonable concentration and at a settled foam quality (%air/%surfactant). After selecting a suitable foam parameter for the injection, we assess injection of pre-generated foam. The injection of pre generated foam does not require pre saturation of the porous media by surfactant. In terms of risk assessment, this type of injection could avoid the solubilization/mobilization and the spreading of DNAPLs into groundwater which is a problem for other injection methods such as Surfactant Alternating Gas (SAG) or co-injection. Series of experiments are performed each utilizing a different scale of the porous medium, ranging from 1D column tests to a 2D pilot test, to a 3D field study. In order to assess the long-term behavior of the foam, that is the development of the foam's blocking ability over time, we develop a simple method and validate it at two different scales (pilot scale and real site). A comparison of two factor is discussed: Resistance Factor RF (translated at same total flow rate, the pressure needed to inject foam over the pressure needed to inject water) over Relative Permeability kr.(corresponding at the relative permeability of water in a two phase system).

1D column test gives good results in terms of foaming ability of the commercial surfactant solution. Good foaming performance was found in the 1D column tests using the commercial surfactant solution. Several concentrations and foam qualities were screened and show two states: weak foam (RF <10) and strong foam (RF<10). In order to increase the volume of foam generated over the time in regard of the pressure constrain, it seems that pre generated weak foam followed by Surfactant Alternating Gas (SAG) is a good alternative as it lowers the required injection pressure compared to just injecting pre-generated foam. In case of pre generated strong foam, the 2D pilot test shows that foam injection requires several pore volume of injection to be effective in terms of reducing global mobility. 1D column test and 2D pilot test results match together in terms of strength and blocking ability of the foam.

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Polymer reinforced foam: influence of polymer composition

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Foam is found in various application fields involving flow in porous media. In petroleum engineering, foam can be used for drilling acid diversion, EOR or conformance control. In environmental engineering, remediation of polluted soil can be achieved using foam. In all these applications stable foams are required to optimize the process. If foam shows several advantages due to its ability to reduce the gas mobility, the weaknesses are related to its instability in presence of hydrocarbons or solid particles and its limited life-time. Several authors proposed to stabilize foams by using water-soluble polymers together with surfactants. Experimental observations have shown that if foamability of the blends decreases slightly, stability was substantially improved [1]. The effect of polymer is mainly to decrease film drainage and increase bulk viscosity of the film. The choice of surfactant and polymer and the concentration of each are crucial to control the polymer reinforced foam flow in porous media. The objective of our study is to compare the effect of different polymers, nonionic and associative, on foam generation, propagation and stability in porous media. The nonionic polymer is a classical PAM while the associative polymer consists in an anionic acrylamide/acrylate backbone bearing a small content of a cationic hydrophobic group. We performed a systematic study of foam flow in sandpacks followed by a waterflood to determine the effect of polymer type on the resistance factor (RF) and the persistence of foam. We show that, due to its composition, the associative polymer is much more efficient to stabilize foam than a classical nonionic polymer especially when surfactant concentration is very low. Then the obtained results were phenomenologically explained by the interplay of the viscosifying effect of polymer backbone and surface activity of hydrophibic groups.

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Shear thinning foam injection as a remediation strategy for NAPL source zone

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The use of foam is promising for the remediation of NAPL-contaminated source zones . Foam has the advantage of reducing interfacial tension and increasing viscous forces while using less surfactant than micellar solution flooding. In addition, air produced by foam favors volatilization of NAPLs. A methodology for surfactants selection suitable for foam production was developed using two critera: Foamability evaluated by the Ross Miles test and interfacial tension reduction measured (against p-xylene) with the Pendant Drop technique. The suitability of the surfactant tested was further assessed by the observation of foam injection conditions in sand columns. Ammonyx Lo which exhibited a low interfacial tension with p-xylene, a high foam height and a stable front when injected in a sand column was selected. In order to produce a stable and viscous foam front a foam production column is needed to make the foam and a pre-flush of the porous media with the same surfactant solution (to make the foam) must be done prior to foam injection. The ability of the surfactant to enhance mobility control and p-xylene recovery in a 2-layer porous media was investigated through a 2D sandbox (2.5 L) experiment containing a coarse quartz sand above a medium sand (permeability contrast of 3). The foam produced with the selected surfactant at 0.1% (w/w) was injected in the sandbox under uncontaminated and contaminated (residual p-xylene saturation of 0.17) conditions. Foam injection under uncontaminated conditions presented a S-shaped front related to shear thinning behavior. During foam injection, complete sweep of the sandbox was achieved with 1.8 pore volume (PV: one PV = 550 mL) compare to 2.8 PV with a conservative tracer. Pre-flush of the contaminated sandbox with surfactant solution initiated p-xylene mobilization but no recovery of free phase. P-xylene was completely recovered in the sand following foam injection. The recovery mechanisms observed were 19% by mobilization, 16% by dissolution and 65% by volatilization indicating the potential use of foam for the remediation of LNAPL source zones.

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Study of foam generation and propagation in fully characterized physical-model fracture

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Foam greatly reduces gas mobility for gas Enhanced-Oil-Recovery (EOR) projects. It substantially increases both the effective viscosity of gas and gas trapping (Ferno et al., 2016). Numerous studies have been conducted to understand foam rheology in rock matrix both theoretically and experimentally. The knowledge of foam flow in fractured porous media is not complete. This study aims towards contributing to the understating of foam generation and propagation in a fully characterized physical-model fracture. The model fracture consists of a rough glass plate, which represents fracture wall roughness, and a top plate that is smooth to enable the analysis of bubble size and to allow direct observation of foam generation (Yan et al., 2006). We experimentally estimate the hydraulic aperture and determine the degree of roughness and correlation length using a surface profiler. The fracture surface was fully characterized and statistically analysed, and a 2D network map was generated from this data (AlQuaimi & Rossen, 2017). First, we investigate the aspects of in- situ foam generation mechanisms and the propagation of pre-generated foam. Second, we benchmark the effectiveness of foam injection in reducing gas mobility compared to gas injection and co-injection of gas and water. Third, we perform foam-quality scans using both in-situ and pre-generated foams at the same flow conditions. Finally, we capture images during transient and stabilized conditions for analysis of bubble size. The study shows that gas mobility is greatly reduced as a results of in-situ foam generation. Foam-generation mechanisms similar to those seen in 3D porous media were observed on this model fracture. Foam was generated predominantly by capillary snap off and lamella division. The injection velocity and gas fractional flow dictates the generation mechanism. Fracture wall roughness played an important role in foam generation. In the case of pre-generated foam, two very distinctive bubble sizes were injected to compare foam behaviour: fine-textured bubbles much smaller than the roughness scale and coarse-textured foam with bubbles much larger than the roughness scale. The first case did not show any significant change in bubble size as foam propagated through the fracture, while the second case showed that the fracture played a role in reducing bubble size. We cannot confirm that foam reached local equilibrium in either case but we believe that it lies between the two cases of in-situ- and pre-generated foams.

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The Effect of Trapped Gas on Foam Flow in a Model Porous Medium

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Gas trapping is an important effect in Water Alternating Gas (WAG) and Foam injection processes. Foams for enhanced oil recovery (EOR) can increase sweep efficiency [1,2], as they decrease the gas relative permeability, mainly due to gas trapping. However, gas trapping mechanisms are poorly understood. Some studies have been performed during corefloods [3], but little work has been carried out to describe the bubble trapping behaviour at the pore scale. Microfluidic experiments are a useful tool for studying the foam flow behavior at the pore scale [4,5]. We have carried out foam flow tests in a borosilicate-glass micromodel with a plate separation of 5 µm. The micromodels were etched with an irregular hexagonal pattern, with a Gaussian distribution of pore diameters (mean = 60 µm) and throat widths (mean = 13 µm) (Figure 1a). Images analysis of the foam flow allowed the bubble centres to be tracked and local velocities to be obtained. It was found that the flow in the micromodel is dominated by intermittency and localized zones of trapped gas. The quantity of trapped gas was measured both by considering the fraction of bubbles that were trapped (via velocity thresholding) and by measuring the area fraction containing immobile gas (via image analysis, Figure 1b). A decrease in the trapped gas fraction was observed for both increasing total velocity and increasing foam quality. Increasing the flow from 10 µL/min to 90 µL/min caused the trapped gas fraction to drop from 59% to 11%. The effect of the foam quality is less strong. Calculations of the gas relative permeability were made with the Brooks Corey equation, using the measured trapped gas saturations. The results showed a decrease in gas relative permeabilities, and gas mobility, for increasing fractions of trapped gas. It is suggested that the shear thinning behaviour of foam could be coupled to the saturation of trapped gas.

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Control of drying with suspensions in porous media

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Interstitial fluid in a porous media is usually not a pure liquid but contains dissolved ions and suspended particles. It is well known that simple liquids evaporate from porous media at a constant rate over a rather long period due to capillary “re-equilibration” allowing a renewal of liquid around the free surface of the sample. Here we discuss the impact, of the presence of particles in suspension in the liquid, on the drying rate of the porous medium. In that aim we in particular rely on the information obtained from Magnetic Resonance Imaging measurements of the liquid distribution in time, and even in some cases the particle distribution. We show that generally in presence of elements in the liquid, the drying rate decreases continuously. With dilute suspensions the elements are transported towards the main interface of evaporation (close to the free surface of the sample) where they tend to accumulate. The drying rate can be exactly predicted by assuming that the liquid evaporates from below this zone and diffuses up the sample free surface. More complex effects appear when the elements are soft microgel particles themselves able to dry but the same migration of particles toward the free surface occurs. When the initial suspension is concentrated, water flow is inhibited and evaporation is controlled by water vapor diffusion.

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Drying-induced salt crystallization dynamics in sandstone: a pore-scale study by 4D laboratory X-ray micro-CT

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Salt crystallization causes major weathering of building stones and landscapes, affects the salinity of soils, and the permeability of reservoir rocks in the context of CO2 sequestration. In all these cases, crystallization is often a drying-induced phenomenon. Theoretical and numerical models have been developed to describe salt crystallization kinetics, pore filling by salt crystals precipitating as subflorescence in porous media, and salt crust development by salt efflorescence on the exterior surface of a porous medium. Experiments have been conducted concurrently on model porous media (e.g. in sand or glass beads packs, and model capillaries [1]-[4]), but direct experimental studies in geomaterials of the governing processes at the pore scale are however limited.

We will present data on the kinetics of drying and deliquescence, and on the concomitant kinetics of salt precipitation and dissolution of halite crystals within the pore space of Mšené (Prague) sandstone, as derived from quantitative image analysis on laboratory X-ray micro-computed tomography (µCT) scans. For that purpose, climatic chambers were developed at the Ghent University Centre for X-ray Tomography (UGCT), compatible with the centre's high-resolution X-ray micro-tomography scanners. This allows for inducing crystallization or dissolution under controlled temperature and relative humidity, and for dynamically visualizing the related ongoing phenomena in geomaterials, by simultaneously imaging the transport and crystallization process during continuous or intermittent scanning. Mšené sandstone samples of 8 mm in diameter were initially capillary saturated with a saturated NaCl-solution and subsequently dried at 20% RH and at 50% RH, at room temperature. These RH-values are representative for winter and summer conditions for NaCl, which is not temperature sensitive. At 20% RH, the dynamics of the formation of a salt skin are quantified, partially closing the pores and causing a slower drying during the continuation of the process. At 50% RH, a constant drying rate and a constant salt growth rate is found during the full drying period. Furthermore, X-ray µCT scans were acquired during subsequent cycles of deliquescence, i.e. exposure to 100% RH, and drying at 20% RH. The humidity cycling causes a migration of the

salt in the subsurface, which is coupled to changing drying kinetics with respect to the first drying of the sample [5]. The quantification of the transport and crystallization dynamics starts from a differential image analysis of the µCT scans [6] in order to discriminate between air, salt solution and salt crystals within the pore space of the sandstone. A pore network extracted from the stone's pore space is subsequently coupled with the differential images [7] in order to characterize drying/deliquescence and precipitation/dissolution events at the scale of each individual pore and to link this with the pore network's connectivity.

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Experimental Studies on Evaporative Drying and Salt Deposition in Porous Media Using Micromodels

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Studies on evaporative drying from porous media are essential for many engineering and science processes, as it is important for environmental and industrial applications such as groundwater and soil remediation, food processing and preservation, and building materials. It is also important in geological applications such as carbon sequestration and the recovery of volatile hydrocarbon from underground reservoirs. Most available literature on drying experiments on artificial porous media have focused on single capillaries or sand packs. We have carried out evaporation studies on a 2.5D etched-silicon/glass micromodel based on a thin section of a carbonate rock, sucrosic dolomite. We employed pore scale visualization to investigate evaporative drying and the associated salt deposition of brine in porous media at different wetting conditions.

We saturated our micromodel with NaCl solutions at concentrations of 0 wt% (deionised water), 18 wt%, and 36 wt% (saturated brine) and passed dry air across a vertical fracture in front of the micromodel matrix for evaporative drying. A technique for wettability alterations of micromodel was developed in-house. The technique involves injecting a solution containing silicone caulk and a mineral spirit (Dodecane) into a micromodel initially saturated with water and then dried before use. Experiments were carried out at different porous media wetting conditions: water-wet, mixed-wet, and oil-wet. During drying the area of the pores occupied by gas/vapor (equivalent to the mass lost by evaporation) was estimated by image analysis.

For deionised water, we observed the three classical periods of evaporation expected from earlier drying experiments in porous media: the constant rate period (CRP) in which liquid remains connected to the matrix surface, the falling rate period (FRP) and the receding front period (RFP), in which the capillary connection is broken and water transport becomes dominated by vapour diffusion. Also, when brine was dried in the water-wet micromodel we observed that the length of the CRP decreased with increasing brine concentration and became almost non-existent for 36 wt% NaCl solution (saturated brine), see Figure 1. However, the length of the CRP for the oil wet micromodel was much smaller with a much prolonged FRP over a larger liquid saturation range.

For all wetting conditions, in the experiments with brine, the dry area of the matrix became linear with the square root of time after the short CRP, as is shown in Figure 2. However, this is unlikely to be due to capillary disconnection from the surface of the matrix as is usually the case for deionised water drying, as the salt crystals continued to be deposited almost preferentially in the channel above the matrix. We propose that this behaviour is due to a combination of salt deposition in the vertical channel and at the matrix surface greatly impeding hydraulic connectivity to the evaporating surface as well as the high viscosity of the saturated brine increasing the viscous resistance to flow.

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Formulation of innovative poultices for the decontamination of porous materials by liquid transfers

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The dismantling of nuclear plants requires different operations including effluents decontamination (liquid treatment) and solids decontamination (surfaces treatment). Porous materials and more particularly cementitious materials (90 % in volume of the contaminated materials) are among the most problematic. Indeed, contaminants tend to incorporate and diffuse into porous structures. Therefore, radioelements (mainly U, Cs, Co and Sr) can reach depths over a few millimeters until centimeters. Today, the conventional techniques of surface decontamination (mechanical, electrochemical or chemical processes) are not suitable for the decontamination of these porous materials.

The aim of this study is to develop an innovative process for the decontamination of porous materials deeply contaminated by radioelements. This process should be simple to implement and has to generate a minimum of treatable secondary waste volume. The chosen orientation consists in developing a process based on the use of poultices. This technology is currently mainly used for the desalination of masonry structures in the field of architectural heritage conservation [1]. Wet poultices are applied to the porous material to be treated and are kept in place during a certain time before being removed. The efficiency of this type of process is related to two factors: first, the capacity of the decontaminating liquid initially present in the poultice to penetrate the porous network of the material and solubilize radioelements and, secondly, the ability of the poultice to re-absorb the solution during the drying stage, as a result of the usual capillary re-equilibration effect, and thus extract the contaminant.

Nuclear Magnetic Resonance (NMR) appears to be an accurate, non-destructive and reliable method to determine transient moisture distribution during various transport processes [2]. Therefore, NMR is used in this study to characterize the moisture transport (allowing the decontamination step) between the poultice and the porous substrate during the different stages of the process: imbibition then drying. The following parameters are estimated for each poultice formulation: decontamination efficiency, depth to which this can be achieved, and time scale required. On the basis of these results, a link between poultice formulation, its physicochemical properties and the decontamination efficiency can be formulated.

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Granular medium surface heave due to internal sodium chloride crystallization induced by evaporation

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The aim of this work is to study the surface heave due to internal crystallization of salt during the drying of a granular porous medium formed by a random packing of hydrophilic glass beads in contact with a layer of hydrophobic glass beads and with a load of polystyrene or stainless beads on top. The hydrophilic packing is initially saturated by a sodium chloride solution. As a result of drying subflorescence forms at the interface between the hydrophilic and hydrophobic layers and then develops within the hydrophobic zone. The subflorescence development leads to a significant surface heave of the granular media assembly. The results indicate that the lighter the load the greater the amplitude of the surface heave. Expressing the balance between the weight of the displaced beads and the force due to the crystal growth allows us to determine the supersaturation order of magnitude needed to obtain the observed surface heave. A simple model taking into account the main phenomena at play is then presented to qualitatively explain the observed phenomena.

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Influence of surfactants on drying kinetics and salt crystallization in porous media

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Salt crystallisation in the porous building materials of historic monuments and statues is being largely recognized as responsible for their deterioration and breakdown. Out of many terrestrial salts, NaCl, being very abundant in the surrounding is one of the major players in salt damage. It has been shown in recent studies that in confined spaces, NaCl crystallizes only after reaching high supersaturations1, which actually increases its potential to exert crystallisation pressure and consequently lead to more damage. In order to mitigate the damage, various remedies are tried, one of which includes the use of crystallisation modifiers2. Different types of additives are known to modify the crystallisation process of NaCl3. These modifiers can also be utilized to change the pattern of crystallisation in a way which makes it crystallize outside the pores (efflorescence) and hence cause less damage. We present both macroscopic and microscopic experiments assessing the impact of various type of surfactants (cationic, anionic, and non-ionic) on the kinetics of NaCl crystallization during evaporation and its direct consequence on the kinetics of drying in sandstones of different porosity. The experiments are done in isothermal conditions at two different relative humidities representative of the summer and winter conditions. Our results show that the addition of small amounts of cationic and non-ionic surfactants drastically change the kinetics of crystal growth. The later leads to salt crystallization as thick crust tightly attached to the surface in contrast to the formation of cauliflower like structures which can be easily removed by brushing when only pure salt solution saturates the stone. In addition, such change in the crystallization process has a significant impact on the drying kinetics by decreasing the evaporation rate. Consequently, the porous materials remain wet for longer time which can subsequently induce other types of damage, harmful for artworks. Our study shows that although surfactants are known to improve the spreading /wetting properties because of the adsorption at interfaces (i.e. solid/liquid and liquid/air), their use in conservation treatment in the presence of soluble salt should be done with precaution as their impact as crystallization modifiers is more detrimental for salt contaminated porous materials than beneficial.

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Moisture migration in partially saturated porous media under non-isothermal conditions

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Pore scale investigation on the base of a discrete pore network model reveals that moisture migration under non-isothermal conditions can lead to distributions of liquid and vapor phase that are usually not caught with traditional continuum models. The effect of temperature distribution appears even more pronounced in porous media with narrower distribution of the pore widths [1]. The pore network simulations of drying with imposed temperature gradients presented in [1-3] show that morphology of the phase distribution is dictated by the direction of the temperature gradient: a stabilized drying front is obtained when the drying process is realized with a temperature gradient oriented as in a classical convective drying process (with hot open network side and decreasing temperature in penentration direction of the drying front) whereas breakthrough of the gas phase with initiation of a travelling two-phase zone is observed when the imposed temperature gradient is oriented as in a contact drying process (with cold open network side and increasing temperature in penentration direction of the drying front). However, these authors either totally [1-2] or partly [3] neglect the effect of simultaneous condensation and refilling of the empty void space accompanying the evaporation process. More recently, experiments presented in [4] reveal that especially temperature gradients with increasing temperature in penentration direction of the drying front can lead to strong condensation effects with growing and merging of liquid clusters. These experiments reflect the phenomenon of moisture migration from warmer to colder regions as they show that moisture evaporated at the warmer pore network bottom migrates in the vapor phase towards the colder pore network top, where condensation occurs. If the condensation effect is strong enough, the colder zone of the pore network can be refilled, regenerating a continuous liquid phase. This allows for subsequent capillary moisture transfer in the liquid phase, which is orders of magnitude faster than vapor diffusion. This is in agreement with the observation of general greater overall diffusion coefficients generally associated with drying processes under similar non-isothermal conditions. A pore network model, incorporating moisture migration with simultaneous evaporation and condensation, can be adapted to related situations with non-isothermal mass transfer in porous media, as exemplarily shown in the figure below, where the liquid moisture from the bottom of the pore network is transfered through a partially saturated zone. The pore scale simulations can give an insight into the dependency of effective transport parameters on the pore size distribution and temperature distribution and the relevant pore level moisture transfer mechanisms.

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Morphological transitions During the Drying of Nano-suspension Droplets containing Surfactants

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The morphology and surface properties of dried particles emerging from the drying of suspensions are strongly influenced by the general dynamics of the drying process and the properties of the suspension. In this work, a comprehensive series of experiments is conducted to investigate the effect of surfactants on the drying behaviour and morphology of the particles resulting from the drying of nano-suspension droplets. To this end, an acoustic levitator was used to study the drying behaviour of single droplets. The temporal evolution of the actual droplets was recorded using an automatic imaging system and the solid particles produced at the end of drying were investigated by SEM imaging. We demonstrate that the morphology of final dried particles can be significantly altered by the surfactant chain length and concentration. The origin of such morphological differences is attributed to two important parameters, i.e. surface tension driven instability and shifts in the permeability of the porous shell formed as a result of drying of suspensions. A plausible mechanism regarding the morphological transformation of the emerging solid particles is illustrated. This research will offer new insights into the surfactant effects on the morphology of particles produced from the drying of nano-suspensions.

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MRI evidence of capillary re-equilibration processes in drying porous medium

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The basic phenomenological mechanisms of drying of simple systems initially filled with pure liquid are well identified [1]. There is first a (generally long) Constant drying Rate Period (CRP), associated with a homogeneous desaturation of the sample due to capillary re-equilibration processes, which in particular maintains the same vapor density conditions around the free surface of the sample (where the main evaporation takes place in that regime), and thus allows to keep the drying rate apparently constant. This is followed by a Falling drying Rate Period (FRP) and more or less simultaneously the apparition of a heterogeneous saturation profile. This transition has a critical interest in the applications as it marks the beginning of a tendency to water retention and a possible dramatic decrease of the drying rate, because the liquid-air interface of main evaporation penetrates in the sample and the vapor has to diffuse through the growing dry region before reaching the ambient air. From internal visualization (e.g. through Magnetic Resonance Imaging measurements) it appears that this scheme is valid for granular packings with grain diameter down to about 0.1 micron. It remains that the exact conditions for which this FRP starts are not yet well determined and understood, except when gravity effects play a dominant role during the process [2]. Through detailed MRI visualizations we show that after the initial constant rate period a gradient of saturation develops in the wet region along with an inward recession of the dry region. During that stage the drying rate is due to vapor diffusion through the dry zone, slowed down by Kelvin effect for small pores. Moreover the liquid goes on flowing in the wet region towards the dry front, so that the saturation goes on decreasing roughlyy homogeneously. We show that this flow (in the FRP) is not a simple Darcy's flow under capillary effects, it results from a complex capillary re-equilibration over the full sample height. This net liquid flux governs the thickness of the dry region. This means that drying is at any stage controlled by capillary re-equilibration processes. We then study in details the drying of a porous medium with a wide range of pore sizes, through MRI water saturation profiles in all directions and with a good time resolution. We show that the saturation profiles along the axial direction exhibit fluctuations in time of amplitude of the order of that of the mean saturation. Moreover we observe correlations between these fluctuations on a scale equal to the sample thickness. This phenomena confirm that re-equilibration processes develop in the sample with a characteristic lengthscale equal to the sample size.

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MRI of bitumen emulsion drying in porous medium

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The preparation of cold mix asphalts, composed of aggregates and bitumen emulsion, does not require any heating, unlike hot mixtures. Accordingly, they represent a substantial environmental potential. The presence of water however delays the strengthening of the material, which progressively acquires its mechanical properties as the water evaporates. Our objective is to better understand how the mix dries and how this affects the structure and properties of the material.

We followed the mass of a bitumen emulsion and sand mix exposed to a dry air flux along its free surface. The evolution of the saturation deduced from these measurements shows that the drying of a bitumen emulsion in a porous medium is much slower than that of pure water. The drying rate decreases from the very beginning, a result which strongly differs from drying of a pure liquid in a porous medium, but is similar to what has been observed for the drying of colloidal particle suspensions. Magnetic resonance imaging (MRI) enables us to measure the spatial distribution of the two emulsion components in the porous sample during drying. Indeed, due to their very different relaxation times water and bitumen can be imaged separately. Recording the signal of the different types of protons in thin cross-sectional layers located at a given position we obtain the water and bitumen distributions, or profiles, along the sample axis. We observe that the water distribution does not evolve homogeneously: far from the free surface the pores remain saturated while an apparent dry front progresses from the free surface. Furthermore, the drying rate measured is much lower than if water diffusion was simply diffusing over the increasing length of the dry front. Although transport and accumulation of bitumen around the free surface of the sample could induce a decrease of the drying rate, it is not the case here: we observe that the bitumen distribution remains homogeneous throughout drying.

These surprising results led us to consider the drying of bitumen emulsion on its own. MRI measurements during the drying along the free surface of the emulsion show that near the free surface a compacted front of bitumen droplets forms, before progressing in the sample. This phenomenon is accompanied with a significant decrease in the drying rate, which seems to indicate that it is the bitumen emulsion in itself which controls the drying rate in the porous medium.

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Pore-level modelling of flow and mass transfer during evaporation in porous gas diffusion layers of polymer electrolyte fuel cells (PEFC)

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The performance of a polymer electrolyte fuel cell (PEFC) is largely affected by the water which is electrochemically-generated inside the porous gas diffusion layers (GDL) of the cell. Based on the available data for water distribution and saturation in GDLs, numerical simulation of phase change and evaporation at the microscopic level enable the engineers to optimally design such porous structures so as to improve the fuel cell efficiency [1, 2]. In this work, a lattice Boltzmann (LB) methodology is used to model the flow and mass diffusion in a binary air/vapor mixture. A modeling framework is designed, focusing on the understanding of the phase change processes of stationary water in the GDL including the interaction of the pore-level transport with the external driving flow in the cell channel. The evaporation process is modelled via incorporating consistent correlations for the evaporation kinetics on the irregular water-gas interfaces. The numerically obtained evaporation rates are compared against experimental data for the exact same 3D porous GDL samples. Simulations are then extended to investigate the performance of the evaporation as well as to study the sensitivity of the phase change process upon varying the involved physical parameters and under various fuel cell operating conditions.

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Relationship between salt precipitation dynamics and evaporative fluxes from porous media delineated by thermal imaging

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Saline water evaporation from porous media is influenced by transport properties of porous media, properties of the evaporating solution and external conditions. In this work, we investigated the effects of salt concentration on the drying behaviour of a porous medium, its surface temperature and surface precipitation dynamics. To do so, a series of evaporation experiments were conducted using columns packed with sand particles saturated with NaCl solutions of varying concentrations. The columns were placed on digital balances to record the evaporation dynamics and were exposed to metal halide lamps to boost the evaporation. A FLIR thermal camera was fixed above the sand columns to record the surface temperature. We could delineate the effects of salt concentration and crust formation on the general dynamics of the evaporation process. Microscopic analysis of precipitated salt at the surface revealed the complex dynamics of salt evolution at the surface and its consequences on the evaporation behaviour. Our results suggest that the presence of porous salt at the surface causes top-supplied creeping of the solution feeding the growth of subsequent precipitation. This phenomenon significantly influences the drying behaviour which makes the characterisation of the evaporative flux a complex task as the drying rate will be dependent on the evolving pore structure of the precipitated salt at the surface. Besides, using the high resolution thermal images, we could establish appearance and disappearance of cold-spots at the surface of porous media brought about by crust formation and preferential water evaporation through the precipitated salt. This study extends the fundamental understanding of the evaporation of saline water from porous media relevant a variety of industrial and environmental applications, such as soil salinization, preservation of building material and CO2 sequestration.

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The Influence of NaCl Concentration and Textural Contrast on Salt Precipitation in Heterogeneous Porous Media

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Evaporation of saline solutions from porous media is governed by the complex interactions between the transport properties of the porous media, the evaporating solution and the external boundary conditions [1]. In the present study, we have investigated the effects of salt concentration and textural contrast on the evaporation process and salt precipitation patterns from porous media in the presence of a sharp textural discontinuity; a common heterogeneity in natural porous media formed due to the weathering or formation of soil horizons, wind deposition and erosion. We have conducted a comprehensive series of macro- and micro-scale experiments to delineate how the drying curve and precipitation pattern is modified as salt concentration varies from relatively low values to a concentration close to the solubility limit, and for a large range of textural contrasts. We showed that for salt concentrations much less than the solubility limit, the precipitation begins at the coarse-textured part of the heterogeneous porous media (which is a counter-intuitive result considering the preferential water evaporation from the fine-textured part of the heterogeneous surface [2]). However, at close to the solubility limit, precipitation initiates preferentially at the fine-textured part of the heterogeneous porous surface. This behaviour results from the interaction between the transport properties of the porous media and the properties of the evaporating solution. Additionally, using pore-scale images obtained by X-ray micro-computed tomography (CT), we have visualized the dynamics of precipitation in the presence of heterogeneity at high spatial and temporal resolution. The pore-scale results corroborate the mechanisms controlling the precipitation patterns in the presence of textural discontinuities inferred from the macro-scale experiments. For experiments conducted with variable textural contrast, we show that precipitation in heterogeneous porous media starts earlier for a higher contrast, due to the stronger hydraulic connection between the two texture domains. Additionally, we suggest that the presence of porous salt structures on the surface of heterogeneous porous media results in similar evaporation behaviour, independent of the textural contrast [3]. This study reveals the necessity to consider simultaneously effects of the presence of textural contrast and the initial salt concentration for accurate description of salt precipitation in heterogeneous porous media. In addition to the hydrological and environmental applications, the findings of this paper will be useful for the design of porous materials to control salt precipitation. This enables us to localise salt precipitation, which could be relevant to preservation of building materials or historical monuments.

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A Microfluidic Platform for Biodegradable and Environmentally Friendly Chemical Oil Recovery

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The flow of nanofluids in porous media has become a common occurrence in various fields including environmental, medical, and energy sectors. In energy sector, a number of recent studies have shown the potential of nanoparticles (NPs) to be incorporated into injected water in water flooding or be used as stabilizer in emulsion flooding to increase the oil recovery. Although NPs have demonstrated promising results for improving recovery factors in core-scale experiments, there are some drawbacks related to nanofluid injections which make them impractical for the field-scale oil recovery applications. For example, NPs cannot increase the water viscosity as polymers do; they are not effective in reducing the interfacial tension as surfactants; and NPs are generally associated with a high cost of production. In recent years, cellulose NPs have attracted attention for many field of studies including biomedical, energy, and fuel cells. Cellulose is one of the most abundant and low-cost materials potentially suitable for nanofluid-based oil recovery utilization. Here in this work, a sample of Alberta cellulose nanocrystal (CNC) is used as the source of nanofluid for the enhanced oil recovery (EOR) process in a well-designed micron sized pore network structures. We use microfluidic-based reservoir models to investigate the role of CNC-based nanofluid and Pickering emulsions (i.e. emulsion stabilized with solid particles) in mobilizing oil trapped in the micro scale porous media. To compare the static and dynamic behavior of CNC nanofluids in oil displacement, the emulsion formation and the stability are investigated both in microfluidic chips under the flow and in static conditions within pipette tubes. It is demonstrated that CNC nanofluid can mobilize oil from most micron-sized channels while the DI water flows through least resistance pathways, leaving behind a large portion of oil in microchannels. This is consistent with the bulk properties of CNC stabilized emulsions, where the stable emulsions are formed even under low external shearing forces. CNC shows the capability of increasing the water viscosity in the same order of magnitude as polymers do for viscosity augmentation. Also because of the high potential of CNC for surface modification, it has promising synergism effects with different types of surfactant which can improve its surface active agent properties and make it an efficient product for EOR. Our microfluidic approach shows the potential for a green chemical oil recovery method, which is biodegradable and recyclable, and reducing the environmental concerns relevant to common chemical flooding. CNC recovers the residual oil efficiently and can be considered as an ideal alternative for polymers or other costly NPs for chemical-based EOR.

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Experimental and Modeling Study of the Effect of Pore Size Distribution on Mechanical Formation Damage in Water Injection

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To maintain pressure of oil reservoirs, water injection into aquifers plays a significant role. Accurate prediction of fluid flow behavior is a crucial aspect which leading to optimum improved oil recovery (IOR). One of the main issues in conventional simulation of water injection is lack of consideration of pore size distribution in flow equations leading to underestimation of mechanical formation damage which is caused by suspended solids in carried water. This study aims to embed the pore size distribution effect in fluid flow simulation and consequently formation damage analysis and improve the simulation results. The averaged upper scale equations have been used to generalize the micro scale classical deep bed filtration model and to predict the permeability decline and pore size distribution modifications during the water injection period. To do modeling as well as validate the obtained simulation results, laboratory test have been designed. Synthesized magnesium oxide (MgO) nanoparticles used as the suspended solids to investigate stable particle (Fig. 1) movement in porous media and monitor the promising formation damage as well as producing the valid experimental observed data (Fig. 2). The results of modeling show the authentic experimental data obtained by use of stable Nano particles. Nice match with experimental data, the permeability decline up to 50% initial permeability, at capturing probability of 0.7 has been acquired compared to mismatch of the conventional simulation results. The other significant result is determination of modified pore size distribution in each simulation time step based on retention concentrations in each grid cell of porous media as consequence of change in effluent suspension concentration (Fig. 3). The main application of this study is to understand pore size distribution changes in case of formation damage dominated regions leading to modification of the static reservoir parameters, such as porosity and permeability maps, in large-scale simulation.

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Experimental Investigation of Dissipative Processes during Two-Phase Flows

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A fundamental understanding of multiphase flows in porous media is relevant to enhanced oil recovery as well as to the process of CO2 sequestration in hydrocarbon reservoirs and saline aquifers. Recently, we quantified two-phase flow mechanisms in micromodels that represent the pore networks of natural complex porous media [1]. Using micro-Particle Image Velocimetry (micro-PIV), we are able to measure accurately the velocity distributions with a vector resolution of less than 2µm in porous media with a typical pore size of 5-40µm. Moreover, we observe and quantify dissipative events, such as eddies within the aqueous phase. These observations motivated further measurement of interfacial dynamics as well as pore-scale and thin film hydrodynamics in a two-phase flow setting. Following our initial work and [2], [3], [4], we explore the origins of dissipative processes at pore scale and their consequences on the upscaling of rock and fluid properties, i.e. relative permeabilities. Our aim is to understand, characterize and quantify these dissipative effects during two-phase flows using micromodel experiments. We performed measurements during immiscible two-phase flow at a variety of mobility ratios in micromodels composed of alignments of pores of different sizes, Figure 1. Using image processing techniques we track the displacement of the moving interface between both fluids and the velocity distribution for different flow rates and viscosity ratios. The local rate of dissipation of mechanical energy due to viscous forces is measured from the velocity fields and used to aid interpretation of core-scale relative permeability.

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Experimental Investigation on Visualization of Gas Bubble Transport in Porous Media

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This research aims in understanding the gas particles behavior in a porous media filled with oil. Such a phenomenon is seeing in steam assisted gravity drainage (SAGD) for oil extraction [1]. SAGD is an oil extraction technique which two pipes are installed in a reservoir where is considered as a porous medium [2]. The oil viscosity is reduced by injecting a steam flow to the reserve through the injection pipe and then is pumped to the ground through the production pipe. Understanding the steam migration in in the reservoir is important to predict the reservoir behavior and to optimize the process. Some researchers have investigated the air bubble transport in porous media. Such studies are limited to using air or water in the medium [3][4] which cannot simulate the oil properties. The transport and migration of oil and water in a porous media has been studied by imaging [5]. No study has been observed to experimentally investigate the migration of a single gas bubble in a viscous porous media. In this research, an experimental setup is designed to track a single bubble transport inside a transparent porous media. Refractive index matching technique for oil and porous media allows visualized the air bubbles. The shadowgraphy imaging technique is then used to track the bubble transport. A picture of the experimental setup is shown in Figure 1. The setup includes a camera, light source, function generator, transparent channel filled with aqua-beads, injection pump to inject the air and data acquisition system. Glycerol with a high viscosity of 1500 cSt at 20°C is used as the fluid in the porous media which are produced by random distribution of aqua-bead particles. These particles absorb the glycerol and become transparent in the glycerol since the refractive index is matched. Figure 2 shows the particles in glycerol before injecting the air. The air is injected to the media using a syringe pump which allows controlling the gas flow rate and producing a single bubble. The study shows that a single air bubble can be easily trapped in the pores and such a particle typically does not move further on its own as shown in Figure 2. If there is no further gas flow, such a trapped particle may clog the pore until the next bubbles approaches the former one. Once bubbles are agglomerated they make a slug that start to move through the pores in the pressure gradient direction. Figure 3 shows an air slug, in the porous media that moves upward. The study also aims in characterizing the bubble transport in the media and investigate the velocity profiles for such transport. The results of this study can be used to validate the theoretical model on gas transport in a viscous liquid in a porous media.

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Fontainebleau Porous Media: Visualization of Oil Bank in MicroModels

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Microfluidic chips are considered to be a laboratory on a chip platform with many applications. For example; flow control, mixing and reaction, ..etc (Micronit, 2016). In our study, we use MicroNit chips to build a conceptional model for the dynamic behavior of multi-phase oil bank displacement in porous media. The chip has been modeled according to our specs and it will be used to interpret and understand the mechanism of forming oil bank in core flow experiment. Fontainebleau sandstone is selected as being the representing simple clean natural porous medium (Zinszner, 2007). Its mineral composition is mostly Quartz (over 0.995). Its grain size distribution is almost constant, range from 150 µm to 300 µm, despite the considerable porosity change (generally 0.02 to 0.3). First, we image the rock texture and structure of Fontainebleau to understand the grain-framework and pore-framework. From Micro-CTs, MICP, SEM, and thin sections, we measure and calculate the grain, pore and throat size distributions (Figure 1).

Figure 1: Left: Micro-CT, Right: SEM

Then, we construct a 2D porous media microfluidic chip (Figure 2), which mimics 3D Fontainebleau porous media. The main geometry features (pores, grains, tubes and throats) of our porous media has been reconstructed. Furthermore, for this chip, the same wettability is maintained; i.e. water wet in our case. The path length of the fluid flow in the Microfluidic chip is 1 meter. This helps us to monitor the process and the dynamic of forming and breakup of the oil bank for a long fluid path. In addition, we expect this measurements give comparable results to our 1 meter coreflow results. For our chip, we follow the same coreflow experimental protocol as for the sandstone, which is: 1- Saturate the chip with Brine 2- Displace the brine with Oil 3- Waterflood the oil by Brine (remaining oil is the residual) 4- Inject Surfactant to sweep the remaining oil. During the experiment, the Microfluidic chip is put under the microscope to visualize, characterize the flow regimes and monitor coalescence rate of the residual oil droplet. This provides us information on the mechanistic and dynamic to form an oil bank. In this poster, we present the parameters which impact the coalescence rate of oil droplet during the surfactant flooding. Also, we show the characteristics of different flow regimes and the dynamic of the oil bank.

Figure 2: Left: Design of the micromodel chip, Right: Fontainebleau Micromodel Chip

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In-situ drainage and imbibition in carbonate rocks using fast synchrotron-based 4D microtomography

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It is estimated that more than 60% of the world's oil reserves are held in carbonate reservoirs. Due to the complex depositional process and post-depositional modification of porosity, carbonate reservoirs generally exhibit multiscale heterogeneity in terms of porosity and permeability. This has motivated many researchers to study flow in carbonate rocks. Thanks to the recent advances in imaging technology, the dynamics of multiphase flow in porous media can be visualized with a high spatial and temporal resolution [1-3]. In this study, we utilized advanced synchrotron X-ray tomography to investigate the dynamics of immiscible two-phase flow in heterogeneous carbonate pore network in 4D. The experiment was conducted using a low-energy beamline (I13) at the Diamond Light Source, Harwell, UK. The sample was initially saturated with water, before a mixture of equal parts of iododecane and dodecane was injected. Following this drainage cycle, imbibition was conducted by injecting water to displace the oil. The exposure time was 0.02s per projection, and 800 projections were captured for each scan with a voxel size of 1.125 microns. The whole experiment ran for almost 10 hours, from which more than 850 three-dimensional images were reconstructed. The high temporal resolution achieved during this study (~40 seconds per scan) allowed for the continuous injection of the displacing fluid meaning that the complex interactions between fluids and pores were visualised and quantified in real time. Using the measured data, we can investigate the pore-scale processes controlling preferential flow in heterogeneous network of carbonate pores, which ultimately influences the dynamics of oil entrapment as well as oil recovery. Our work extends the understanding of the effect of porous media geometry and heterogeneity on immiscible multiphase flow in complex pore systems. The findings of our research will be relevant to a variety of industrial and environmental applications such as oil recovery from complex carbonate reservoirs, and remediation of non-aqueous liquids from groundwater.

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Influence factors of the foam formation in porous media

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Foam displays a wide application prospect in enhancing oil recovery process. It can control water channeling in water flooding reservoir, and also can inhibit gas channeling in low permeability gas-drive reservoirs. However, there are many questions about foaming ability in reservoir, influence factors of foam formation, screening criteria of foaming agents for deep profile control and so on. There are a number of factors affecting foam generation in porous media. Kanda et al. [1] conducted foam generation experiments in packed tube with glass beads, and reported that good foaming ability, low surface tension and large surface viscosity favor foam formation. ISLAM et al. [2] observed that there was an optimum surfactant concentration for creating foam. Rossen et al. [3] discussed the influence of pressure gradient on foam generation, and derived an expression of the minimum pressure gradient. The objective of this work is to study effects of slug size of liquid and gas, gas: liquid ratio, injection rate, permeability, pressure and properties of foaming agents on the formation of foam in porous media, and examine the conditions under which foams can be created in reservoir. Foam was generated by alternating foaming agent and nitrogen in core flood. Experiments were carried out using a range of man-made quartz cores with 10cm in length, 2.54 in diameter, average permeability varied from 100mD to 1000mD. Using short core was to neglect the loss of foaming agent and distribution of foam formation along the core. Three kinds of foaming agents were screened according to their different foaming ability and foam stability in static bulk foam test. The first one was a mixture of 0.3%wt of Laurel amide propyl amine oxide (LAO) and 0.5%wt of Dodecyl dimethyl amine oxide (OA-12) with better foaming ability and weak foam stability; the second one was 0.8%wt of Dodecyl hydroxypropyl sulfo betaine (Z-12) with good foaming ability and good foam stability; the third one was a mixture of 0.3%wt of LAO and 0.5%wt of Fatty alcohol polyoxyethylene ether sodium sulfate (AES) with weak foaming ability and better foam stability. The injection rate varied from 1.5 m/d to 15 m/d; gas: liquid ratios were 1:2, 1:1 and2:1. At a fixed injection volume 36 PV of liquid and gas, slug size varied from 0.1 PV to 0.6PV, and back pressure varied from 0.3MPa to 4MPa. The effectiveness of a foaming agent creating foam in porous media was determined by measuring its produced foam volume and resistance factor. It was found that the produced foam volume in cores is much less than that in static bulk foam test. Resistance factor is increased by increasing permeability (Fig1.) and back pressure. There is an optimum value in injection velocity, slug size, and gas: liquid ratio. The experimental results also showed that foaming agent with better foam stability have higher resistance factor than that with better foaming ability (Fig.2).

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Introducing a complementary method for efficient pinpointing of MMP measurement for gas hydrocarbons in gas injection process

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Accurate experimental measuring of minimum miscible pressure parameter in gas injection scenarios is always demanding but crucial and problematic test. By the passage of time, different methods have been raised but there is no complete agreement on experimental pinpointing of this important parameter. In other words, the results are always depends on final recovery factors measured roughly in each pressure steps. This experimental research aims to introduce the results of slim tube experimental set up commingled with continuous high pressure density meter. Using this complementary device, effluent high pressure phase density was measured continuously and the density curves were interpreted precisely in each pressure step. The results showed that coming close to minimum miscible pressure leads to appear a new transition zone in density- pressure curve which is so called mixed density zone. In this experimental research constructing of density profiles of effluent phase for an Iranian oil field have been targeted. Using these handy profiles one can determine precise estimation of MMP and figuring out true miscible or immiscible pressure steps.

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Investigation of EOR Processes and their impact on Oil Recovery using Pore Network Modelling Techniques

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In this work, we describe a new dynamic pore network model that has been developed to investigate a wide variety of EOR techniques and their impact on oil recovery. The model operates under unsteady-state flow conditions, where viscous forces may no longer be considered negligible compared to capillary forces, and a full range of wettability states – including mixed-wettability – are included. We introduce a novel formulation, where fluid fractions are updated in capillary elements according to the relative balance between capillary and viscous forces. Film transport has been also considered in the model, and a tracking algorithm has been implemented to follow the flow of low salinity water and/or polymer during secondary and tertiary flooding.

The model is completely general and can consider multiple phases flowing under various injection protocols and we show that such an approach is able to reproduce a wide range of experimental observations. The model is easily adapted for any network model architecture and results are presented from off-lattice, rock-derived networks of sandstone and Berea samples.

We have investigated the impact of several parameters on numerous secondary and tertiary EOR recovery processes. The effects of injection flow rate, oil and water viscosity, network geometry (pore size distribution, network connectivity, inter alia), initial water saturation and network wettability have all been studied and compared to experimental results from the literature.

We show that both low salinity water injection and polymer injection can lead to an increase in oil recovery under specific conditions related to the flow regime, the water viscosity change and the rock wettability change. We also show how the efficiency of these EOR techniques depend upon whether they are applied during secondary or tertiary floods. The effect of the timing of various EOR techniques has been also investigated.

Finally, we present recovery data from low salinity polymer injection simulations, where system wettability and water mobility are varied simultaneously. Results suggest that the synergy between these two EOR processes affect sweep efficiency at the pore scale, yielding additional oil recovery.

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Micro-scale experimental investigation of the impact of surfactant structure on the residual trapping of non-wetting phase in natural porous media

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Residual trapping of a non-wetting phase in a porous medium is directly impacted by the relative magnitude of capillary, viscous, and gravity forces. Parameters such as pore geometry, rock surface wettability, fluid-fluid interfacial tension, fluid viscosities and densities, and fluids' flow rates determine the magnitude of the above-mentioned forces. Ratios of the forces control the sequence by which different pore-scale displacements take place, which in turn determines the pore-scale fluid occupancy and the residual non-wetting phase saturation. In this work we show that there is an additional set of factors that directly contributes to how fluids are distributed at the pore scale. We show that under similar rock and fluid properties, interfacial repulsive and attractive interactions, caused by the adsorption of surface-active chemicals on fluid-fluid interfaces, can significantly alter micro-scale fluid occupancies. In this work, these effects are created using two surfactant structures (nonionic and anionic). We investigate the impact of surfactant structure on pore-scale fluid distributions in a miniature limestone core sample subjected to injections of different wetting fluid solutions.

Using micro-computed tomography (micro-CT) imaging technique and miniature core-flooding methods, we directly visualized pore-fluid occupancies in a miniature limestone rock sample subjected to oil-displacing-brine (drainage) and brine-displacing-oil (imbibition) flow tests. The core plug was imaged at the end of drainage (i.e., at initial water saturation (Swi)), and at different stages of imbibition (i.e., at different intermediate (So) and residual oil saturations (Sor)). The images were generated at a voxel resolution of 2.3 µm3. A nonionic surfactant and an anionic surfactant were utilized as surface-active agents. Theses surfactants provided similar IFT values of 6.56 ± 0.07 and 4.24 ± 0.02 mN/m and analogous in-situ contact angles of 41.99◦ ± 6.58 and 37.73◦ ± 6.80, respectively. The calculated capillary numbers at the end of imbibitions were comparable with an average value of 2.84×10-6. We measured porosity, oil saturations, cluster-size distribution, cumulative volumes, surface areas, and shape factors of the residual oil phase in the porous medium.

Oil cluster analyses along with three-dimensional visualization of fluid distribution indicated that using the nonionic surfactant instead of anionic surfactant resulted in breaking off the large and medium oil clusters to smaller and more scattered globules. This improved the frequency of pore-body filling displacement mechanism compared to snap-off. We observed that during the imbibition in the presence of nonionic surfactant, brine started to displace the oil at much earlier stages of flow process (0.3 pore volume injected (PVI)). The results also show that the residual oil saturation reduced by 18% in the presence of the nonionic surfactant under similar Swi compared to that of the test with no surfactant present (blank brine injection). While, the displacement of oil phase by the brine solution that contained the anionic surfactant reduced the trapping only by 8%. We propose a mechanism relating the stability of oil-brine interfaces to surfactant structure that is responsible for break-off and/or coalescence of oil clusters inside the pore space. The suggested mechanism was confirmed by micro-CT images and associated oil cluster analysis.

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Microscopic configuration and deriving mechanisms of residual oil after water flooding in porous media

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Currently, most of the onshore oilfields in China have been highly flooded with water, which make it more and more difficult to recovery the remaining oil for economic development. In order to improve the oil recovery from these mature fields, fully understanding of the microscopic configuration and driving mechanisms of residual oil after water flooding is required. In this work, we firstly analyzed the flow characterization and residual oil microscopic configuration after waterflooding using microscopic model. The results show that both capillary and viscous forces control the residual oil distribution after water flooding, and the remaining oil, based on the microscopic configuration, could be classified as no sweep region, the cluster type, the columnar type and the isolated island type. Based on the apparent wetting contact angle, we then formulate a correlation between wettability index and the contact angle; this allows us to calculate capillary force quantitatively in the reservoir condition. Through the comparison of the capillary and viscous forces for the different classified types of residual oil, the main control force and starting mode of different types of microscopic residual oil in Daqing oilfield were studied. Finally, the indoor oil displacement experiments using microscopic model and one-dimensional natural core samples were performed with different pressure gradient and different fluids systems, such as ASP and SP systems. The results show that, in the weak and non-swept areas, the residual oil is primary exist as long-capillary form, namely no sweep region and the cluster type. A higher displacement pressure gradient should be applied to recovery this type of residual oil. While, in the high flooded areas, the remaining oil coexist as long-capillary (cluster type) and short-capillary (discrete type), and it could be remobilized by increasing the viscosity of displacing phase, enhancing the displacement pressure gradient and reducing the interfacial tension.

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Modeling of nanoparticle retention and transport for heavy oil viscosity reduction applications

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Recent pilot studies in Colombian reservoirs have demonstrated the benefits of nanotechnology at improving heavy oil mobility, due to both wettability alteration and viscosity reduction. Understanding the physical and chemical processes that occur in the reservoir during the injection/production of nanofluid is essential for the design of the stimulation operations. In this work, we study the use of nanotechnology for increasing mobility of the heavy oil. A mathematical model is proposed for studying the behavior of nanoparticles injected into the reservoir. Adsorption of asphaltenes on the surface of the nanoparticle and their effect on the viscosity of crude oil is accounted for in the model formulation. In addition, nanoparticles are retained/mobilizazted as operating condition changes. The transport and retention models are coupled to a multiphase/multicomponent model. The finite volume method is used to solve the differential equations of the model, following a second order discretization scheme. The resulting equations are solved using the Newton Raphson method. Laboratory tests were used to calibrate and validate kinetic parameters of the model. Subsequently, the model is validated with results at field scale, an application was implemented in a set of wells of a Colombian field, located in the Llanos basin. The intervention jobs were designed within a treatment radius of approx. 3 ft, pumping 86 Bbl and 107 Bbl of nanofluid as main treatment in well_A and well_B respectively. After the jobs, the production of the wells showed instantaneous oil rate increases of around 310 bopd in well_A and 87 bopd in well_B, not BSW reductions were observed. The results of the simulation adequately reproduced the production rates and cumulative volume of oil during stimulation operation, the maximum error found does not exceed 10%. With the numerical simulations, it is possible to predict the evolution of the nanoparticles in the reservoir, in addition to quantify the content of asphaltenes retained in the matrix and adsorbed by the surface of the nanoparticles. The oil recovery factor can be estimated for a given well intervention using the proposed mathematical model, which can be used for nanofluids deployment optimization procedures.

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Nanoparticle-enhanced immiscible fluid displacement in porous rocks

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The present work investigates multi-phase fluid transport in porous media at pore-scale, specifically, the effect of nano-particles (NPs) aqueous suspensions in remobilisation and recovery of trapped organic fluids from a carbonate rock with a multi-scale pore-structure. Our findings have implications for a wide range of applications including: (i) remediation of aquifers contaminated by non-aqueous phase liquids (NAPL), (ii) oil recovery from hydrocarbon reservoirs, and (iii) storing CO2 in the geological formations (CCS). Recently, use of NPs in groundwater remediation has been extensively researched, with studies both performed at laboratory and field scale (Zhang et. al, 2006), it has been shown that immiscible displacement of organic fluids from porous media can be enhanced in presence of NPs. The main mechanisms identified are (i) reduction of fluid-fluid interfacial tension (IFT), and (ii) wettability alteration from oil-wet to water-wet or mixed-wet. Traditionally, core-flooding experiments are used to study the effectiveness of introducing a third phase, such as an aqueous phase that contains nanoparticles, or surfactant or a combination of the two, in removing oil from porous media. However, although useful in understanding the results of flow processes, such indirect methods are limited in establishing the details of governing mechanisms at the scales they occur, i.e. pore-scale. Hence, fundamental research questions remain open demanding use of advanced technologies such as X-ray computed micro-tomography (µCT) to investigate parameters involved in NPs-induced recovery enhancement through in-situ imaging of fluid displacement dynamics. Designing a successful NPs-based organic phase recovery involves deciding on the NPs type, size, concentration, surface and bulk properties (e.g. wetting and magnetic properties), salinity of the carrier aqueous solution (impacts the stability of the NPs suspension), and possibility of adding surfactants for synergic enhancement of oil removal. Using µCT-monitored core-flooding experiments and hydrophilic SiO2 NPs we examined the effect of particle concentration on enhancing the recovery of a mineral oil from a water-wet dolomite. The investigated concentrations were 0.05 and 0.1 wt% and the fluid displacements were performed under capillary-dominated flow regime to mimic the flow dynamics of oil reservoirs. The core was initially saturated with water, followed by oil injection and NPs suspension injections. A 3D image was collected after each injection step, using an X-ray transparent fluid flow cell (Pak et al., 2015) integrated with the µCT instrument built in University of Edinburgh (Figure 1A). Our experiments show oil remobilisation occurs only at the higher NPs concentration. The pore-scale distribution of the organic and aqueous fluid phases indicate the rock wettability has remained unchanged, i.e. water wet. Instead, we, for the first time, observed an in-situ formation of an oil-in-water emulsion, stabilised by the NPs, consistent with Pickering type emulsions (see Figure 1B). A reduced IFT, induced by NPs, assisted formation of emulsions through roof-type snap of events. The emulsion is only observed to have formed within the pores with high aspect ratio, i.e. the vugs. Our future experiments will investigate the effect of NPs sizes and surface characteristics on formation of oil/water emulsions and enhancement of organic phase recovery.

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NANOTECHNOLOGY EFFECT ON THE RHEOLOGY OF HEAVY CRUDE OIL AND ITS MOBILITY ON POROUS MEDIA AT RESERVOIR CONDITIONS

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The heavy (HO) and extra – heavy crude oils (EHO) are attractive for the oil and gas industry due to their vast reserves but are challenging because their main characteristics of high density and extremely viscosity which difficult the mobility on the reservoir and at surface conditions which affect the production, transport and refining processes. The commonly techniques used to improve mobility of oil to deposits and surface conditions are economically and environmentally costly [1, 2] such as: 1) dilution techniques with several solvent chemicals (toxic) of high volumetric consumption, which requires an intensive maintenance of pipelines and storage systems due to their characteristic corrosives [2, 3] and 2) thermal techniques which are highly costs due to the energy consumption [4, 5]. Recently, the nanotechnology is offered as an emerging technique capable of competing economically and technically against conventional processes due to their unique properties. Due to their particle sizes, between 1 and 100 nm, large available surface area, high dispersability and tunable physicochemical characteristics, nanoparticles are prone to selectively adsorb asphaltenes and inhibit their self-association. Several researchers have demonstrated the application of nanoparticles in several areas of Oil & Gas industry [6-8], which may features the strongly interaction with the asphaltenes and the reduction of the aggregate due to the ability to adsorb them and other molecules present in the HO and EHO, which can positive impact the viscoelastic network of nanoaggregates reducing viscosity of the these type crude oils. In this order, the aim of this paper is to evaluate the effect of nanoparticles on the rheological properties of a Colombian HO at varying conditions of temperature, shear rate and dosage of nanoparticles. The selection of the nanoparticles, optimized towards the adsorption and size reduction of asphaltenes, was achieved using adsorption isotherms and the growth kinetics of asphaltenes. We evaluate the effect of nanoparticles and nanofluids as viscosity reducers for heavy crude oil (HO). The effect of alumina, silica and acidic silica nanoparticles was evaluated through n-C7 asphaltene adsorption and aggregation tests using UV-vis spectrophotometry and dynamic light scattering. The nanoparticles of acidic silica were used to prepare a water-based nanofluid at different concentrations in distilled water, and with the addition of 2.0 wt% of a non-ionic surfactant. The shear rheological response was obtained as function of nanoparticle concentration, temperature (from 298 to 323 K) and shear rate (ranging from 0 to 100 s-1). Experimental results indicate that increasing the concentration of nanoparticles in the mixture, up to 10000 ppm, leads to a viscosity reduction of approximately 90% in comparison with the nanoparticle-free crude oil. At higher concentration of nanoparticles, the effectiveness of the heavy-oil viscosity reduction diminishes. Rheological tests showed a non-Newtonian behavior for the mixtures tested at 298 K. However, as the temperature reaches 323 K the specimens behave in a Newtonian fashion. Coreflooding tests were conducted under typical reservoir conditions of pore and overburden pressures, i.e. 2600 and 3600 psi, respectively, and at 360 K. Results indicate that the addition of nanoparticles increases the heavy oil mobility and leads to an improvement in oil recovery of roughly 16%. The results in

this paper are expected to open a wider landscape on the use of nanoparticles in IOR processes based mainly on “huff & puff” configurations.

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Oil/Gas Production Optimization and Risk Analysis by Developing New Plugin: Using Real Case Study

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Abstract Intelligent well technology has provided facility for controlling subsurface phenomenon. Early recognition of unwanted fluid production allows for rapid remedial action. Effective down hole behavior management will depends on the appropriate performance of intelligent devices in the wells with maintaining the hydrocarbon production based on the predefined criteria over the whole well/field life. However, there is still an incomplete understanding of using intelligent well concept to optimize the different objection functions regarding intelligent well/field attitude and investigation of their application risks effects. The present study will introduce a novel developed Plugin for Interval Control Valve (ICV) performance. This Plugin will allow users to optimize different objective functions with manipulating ICV functionality. The objective function can be, maximizing wanted fluids (oil), minimizing unwanted fluid production (water) or both, simultaneously. A workflow is proposed for the developed Plugin applications based on a predefined subsurface criteria and objective function. For avoiding long simulation run times, a proxy model has been developed and applied. A real case study is considered to demonstrate the effectiveness and robustness of the proposed Plugin. Different intelligent scenarios have been evaluated based on the objective functions. After selecting the best amongst all the possible candidate scenarios, the risk analysis of ICVs has been performed. The optimistic, most likely and pessimistic scenarios have been presented based on intelligent well concept and risk attitude. Results showed the significant improvement in the objective function achieved using the developed methodology.

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Pore-Network Modelling of Transport under Two-Phase Flow in Porous Media

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Enhanced oil recovery comprises injection of chemicals with water to improve the oil recovery from the oil reservoirs. To simulate the transport for enhanced oil recovery, usually the transport of the chemicals is characterized by single-phase transport coupled with two-phase flow [1, 2] which is inconsistent.

In this study we develop a pore-network model to simulation advective-dispersive transport [3] in a three-dimensional pore network for different saturation states. The simulations evaluate the origin of the non-Fickian transport under different degrees of saturations at different Peclet numbers.

Our results highlight the non-monotonic trend of the stagnant saturation versus the total saturation, which highlights the mixing the chemicals with the resident brine. This impact is very important in the efficiency of low salinity water flooding where the mixing of the low salinity and high salinity with reduce the efficiency of the technology.

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Study of the Chemical Flooding Effect in Gao-63 Reservoir

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Because of the chemical flooding has quick effect, good benefits, mature technology and many other advantages, its research and application have been paid more and more attention. At present, the main chemical flooding technology to enhance oil recovery in China are polymer flooding and combination flooding which are studied more and more deeply. They are mature technology in Daqing oilfield and were industrialization promoted. Then we got good effects. In this paper, on the basis of the investigation, application and displacement mechanism about chemical flooding between domestic and foreign status, in view of the Gao-63 reservoir conditions, through the research on the polymer solubility, viscosity, resistance to shear characteristics and interfacial tension of surfactant, we select the best polymer and surfactant for oil displacement and thus to prepare binary and ternary systems. Using physical simulation experiment, we conduct polymer flooding, binary compound flooding and ternary complex flooding oil displacement experiment on Gao-63 core. Then we study the oil displacement effect of different oil displacement system in different reservoir conditions. Finally, in view of the Gao-63 reservoir conditions, we will screen out the best oil displacement system. The results showed that the binary system composed of a polymer concentration of 1000 mg/L ZLPAM2 and a surfactant concentration of 0.3% XPS has better viscous effect and ultra low interfacial tension. Injection 0.3PV binary system 1000mg/L ZLPAM2+0.3%XPS and subsequent water flooding to Gao-63 reservoir simulation core with permeability of 400/1000/2000mD and 200/1000/2000mD, rate of water content significantly decreased and improve the recovery rate of about 30%. As can be seen for Gao-63 reservoir, the recovery efficiency enhancement is not significantly affected by the reservoir heterogeneity, but the ultimate recovery will decrease along with the reservoir heterogeneity increasing.

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TECHNOLOGY FOR ENHANCED RECOVERY BASED IN WATER INJECTION IMPROVED WITH NANOPARTICLES-POLYMER

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Today global energy demand increases significantly, but supply growth does not increase in the same proportion. In particular, the oil industry has been affected by the shortage of discoveries of new deposits of oil, which has led large companies to seek alternatives that allow them to increase the supply of oil. Thus, oil companies have focused on the exploitation of unconventional reservoirs through technologies of enhanced oil recovery (EOR), which are a set of techniques that are intended to improve the flow conditions in the porous medium. One topic of great interesting in these techniques is the water injection, which is applied to improve efficiency through control of mobility in a porous medium, considering that this chemical method has technical and economic limitations that interfere with the success in the recovery of petroleum. For this, the nanotechnology emerges as a good option to solve this problem. The nanoparticles have several properties such as optical, chemical, electrical, thermal and mechanical, that can be interesting in production engineering to enhance activity and contact area. The idea to use nanoparticles in EOR has been recently researching observing features such as interfacial tension reduction (IFT), wettability alteration, thermal conductivity and oil transportation in the reservoir with nanoparticle stabilized emulsions. The most common phenomena observed during the injection of nanoparticles into a porous medium are adsorption, desorption, and transport [1-4]. Therefore, this study aims at improving the current recovery technique using nanotechnology. With a formulation of nanofluid composed by Nanoparticles-Polymer, it is expected to provide a greater viscosifying effect, using a low concentration of polymer (primary component recovery processes), also provide greater thermal stability of the polymer at high temperatures and shear stress when it enters the well. This will avoid rapid degradation and loss of properties, increasing the efficiency of the conditions of the macroscopic sweep, decreasing the fingering problems, and finally, increase recovery rates compared to the conventional technique. To carry out this proposal is followed a methodology that starts with the synthesis and characterization of the nanoparticles to be used in the development of improved water, then this will be tested in dynamic tests in cores at laboratory scale, comparing the results with the traditional technique. Some preliminary results obtained shows the added value by using silica nanoparticles (synthesized under the Sol-gel method) with the polymer, increasing the rates of recovery between 6 to 8 points in displacement tests.

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The impact of heterogeneities on CO2 foam flow behavior in a microfluidic device

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A heterogeneous microfluidic device is fabricated using borosilicate glass and a two-dimensional representation of a Berea sandstone. The porous medium is designed with a central low permeability zone and a high permeability zone on each side of the low permeability area. Water and pre-generated foam are injected into the oil-saturated microfluidic device using various injection rates to examine flow behavior and the impact of foam on mobility control. A 500 ppm blend of surfactants are used to stabilize CO2 foam in the presence of crude oil. The flow pattern of water and foam across the microfluidic device is recorded using a high resolution camera, which enables capturing images of the entire porous medium (approximately 3.5 cm X 4 cm) with the resolution required to discern features as small as 10 – 20 micrometers. The displacement of the resident fluid as a function of pore-volumes injected is presented. Results show that, compared to water, foam displaces the resident fluid more effectively in both high and low permeability regions. This effect is significant in the low permeability region, mainly due to the relatively high apparent viscosity of foam. The resulting resistance to flow in the high permeability region overcomes the entry capillary pressure in the low permeability region and the surfactant solution is thus able to infiltrate and sweep the low permeability region. The foam stays gas-rich in high permeability zones and solvent-rich in the low permeability zone. This study provides evidence regarding the mechanisms responsible for the improved sweep efficiency of the resident fluid using foam compared to water in porous media.

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Three Phase Hydrocarbon Thermodynamic Vapour-Vapour-Liquid Equilibrium during CO2 Displacing Condensate Gas with High Temperature

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Gas-condensate reservoirs are an essentical part of China's hydrocarbon resources. Injectng supercritical CO2 into gas reservoir is a novel trial to improve condensate gas recovery and decrease the hydrocarbon liquid dropout. A good understanding of the effect of supercritical CO2 on the phase behavoir peroperties of these hydrocarbons is essential for accurately forecasting the displacing performance of the reservoirs with numerical simulators.

This paper presents novel phase behavior experimental procedures and phase equilibrium evaluation methodology for a Chinese gas-condensate phase system mixed with supercritical CO2 with high temperature. A unique phase behavior phenomena was also reported. The objective of this work to verify and evaluate the effect supercritical CO2 on enhancing gas recovery of condensate gas reservoir.

Firstly, the new phase behavior experimental procedure was established. The phase behavior of the combination of condensate gas and supercritical CO2 was tested in the apparatus which consists of high-pressure, high temperature, PVT cell equipped with high resolution digital camera. The cell is placed inside a temperature-controlled bath. Under 132℃, the CO2 was firstly pumped into PVT cell and then condensate gas was pumped upward. When pressure drop to specific pressure range, the interfacial phenomena between condensate gas and supercritical CO2 like fine mist or cloudiness appeared in PVT cell were observed and recorded. The thermodynamic properties of different vapour phases were measured. Another important observation is the mass transfer of supercritical CO2 into the condensate gas. The mass transfer time between two vapour phases was also measured.

In order to interpret and identify condensate gas and supercritical CO2 interfacial phenomena, multiphase thermodynamic VVL equilibrium model considering condensate gas and supercritical CO2 interphase was established. The fugacity of gas phase with rich CO2 was calculated by adjusted Peng-Robinson equation of state considering two volume correction adjusted terms considering temperature influence and critical point influence. These terms were adjusted with experiment data. With different fugacity models, gas phase splitting with rich CO2 and condensate gas were carried out.

Finally, taken YKL condensate gas as example, three phase hydrocarbon thermodynamic parameters with CO2 displacing YKL condensate gas were calculated with multiphase thermodynamic VVL equilibrium model, which were consistent with the PVT experiment data. The calculation results indicated that there are VVL Equilibrium zone when temperature is higher than 132℃, CO2 concentration is higher than 55%, pressure is at the range of 20000kpa and 27000kpa.

PVT Experiments and thermodynamic VVL equilibrium model both verify that under a certain pressure and CO2

concentration conditions with high temperature, supercritical CO2 can be used as efficient displacing media to flood condensate gas, where CO2 displacing behavior looked like “cushion gas” and CO2 was not easy to be mixed with condensate gas.

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TRANSPORT AND MIXING OF LOW SALINITY WATERFLOODING IN POROUS MEDIA UNDER TWO PHASE FLOW CONDITIONS

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Transport of low salinity water in sandstone oil reservoirs (Low Salinity Waterflooding) has been experimentally proven to increase additional oil recovery up to 15% of OOIP (original oil in place)[1, 2]. Waterflooding in oil reservoirs leads to two-phase conditions, which causes a development of saturation topology due to immiscibility of oil and water. Saturation topology controls the distribution of immobile (stagnant) and mobile zones (flow contributing areas) and essentially has an impact on the transport of low salinity and its mixing with high-salinity as immobile zones will limit the reach of low salinity to all areas. Transport of low salinity after high salinity waterflooding under two phase conditions and the dispersivity of low salinity is analysed in this study through numerical modelling using Volume of Fluids Methods implemented in openFoam®. Results agree well with the experimental data, as immobile saturation has a non-monotonic relationship with saturation and at intermediate saturation range, the immobile saturation is at highest range [3]. Dispersion coefficient increases with increase of rate of injection with a non-monotonic relationship with water saturation [3].

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Transport Mechanism of CO2 in Fractured Chalk

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The main objective of this study is to develop and test a proper description of diffusion and transport effects in fractured chalk systems with CO2, water and oil. Both experiment and numerical modeling work are conducted in this study. Based on the experiments, simulation models are built to mimic the main transport phenomena, including diffusion which was found to be particularly important. The verified modelling framework can properly account for all the relevant forces: (1) viscous displacement, (2) gravity effects, (3) diffusion effects, and (4) effects caused by changes in interfacial tension (IFT). In this study, we have conducted in total of 11 experiments: (a) Work Package (WP) 1-1 and WP1-6 cover CO2 flooding (CF) into fractured-chalk core saturated with North Sea Chalk Field (NSCF) stock-tank-oil (STO) at zero irreducible-water saturation, (b) first-contact miscibility is studied in WP1-2 for CO2-C10 system, (c) WP 2 is the series of IFT measurements conducted on CO2-STO system at 110 oC, (d) WP 3-1 conducts the water flooding (WF) followed by CF at reservoir conditions in a large outcrop chalk with 26 cm long and 12 cm diameter. The fractured-chalk system is initialized with NSCF live-oil and connate-water saturation. (e) WP 4-1 is identical with WP 3-1 except the system is initially saturated with NSCF STO and connate-water saturation. (f) WP 5-1 conducts similar experimental procedure as WP 4-1 in a composite chalk core, with the total length of 45 cm and average diameter of 3.74 cm. This addresses capillary continuity among all six chalk cores. (g) WP 5-2 is identical to WP 5-1 except the use of synthetic formation water with zero amount of sulfate for the WF instead of sea water with considerable sulfate content. (h) WP 5-3 is identical with WP 5-2 except the use of NSCF reservoir rocks. In all of the experiments, a centralized hole represents the “fracture”. Prior to above experiments, we develop a constant volume diffusion (CVD) experiments (WP1-7 & WP1-8) for STO and live-oil samples that determine the multi component diffusion coefficients at reservoir conditions. In this technique, the system is initialized with an oil-saturated chalk in direct contact with an overlaying open space filled with CO2 (CO2 chamber) at reservoir conditions. Diffusion coefficients are determined by fitting the pressure decline data. Equation-of-state (EOS) is tuned using reported lab PVT data and is employed by numerical simulator. The Parachor parameter in EOS model is further adjusted to match a series of IFT measurements at 110 °C. The tuned EOS assures a good estimation of IFT, phase behavior and volumetric properties for different mixtures of CO2 and oil at reservoir conditions. All experiments are successfully simulated and history matched via numerical modeling by incorporating all the relevant displacement mechanisms. Results shows that active imbibition (strong and moderate type) exists between matrix-fracture system during WF. Moreover, the mass transfer during CF is mainly controlled by diffusion rather than the convective flow or the viscous forces.

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Analytical approximations for effective relative permeability in the capillary limit

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We present an analytical method for calculating two-phase effective relative permeability, under steady state and capillary-limit assumptions. These effective relative permeabilities may be applied in experimental settings and for upscaling in the context of numerical flow simulations, e.g., for CO2 storage. An exact solution for effective absolute permeability in two-dimensional log-normally distributed isotropic permeability (k) fields is the geometric mean. We show that this does not hold for relative permeability since log normality is not maintained in the capillary-limit phase permeability field when capillary pressure, and thus the saturation field, is varied. Nevertheless, the geometric mean is still shown to be a suitable approximation when the variance of log k is low. For high variance cases, we apply a correction to the geometric average gas effective relative permeability using a Winsorized mean, which neglects large and small values symmetrically. The analytical method is extended to anisotropically correlated log-normal permeability fields using power law averaging. In these cases, the Winsorized mean treatment is applied to the gas curves for cases described by negative power law exponents (flow across incomplete layers). The accuracy of our analytical expressions is demonstrated through extensive numerical tests, using low-variance and high-variance permeability realizations with a range of correlation structures.

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Micro-model Experiment on Dilution assisted Solvent Recovery for Heavy Oil

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Dilution assisted solvent recovery for heavy oil has been identified as a potential game changing technique; it has significant improvements over conventional thermal EOR, such as no water consumption, one fifth of the energy consumption and hence a significant reduction in GHG emissions. However several processes occur in the reservoir, such as mechanical dispersion and asphaltene precipitation. Diffusion enables bitumen molecules to move from the immobile zone to the solvent-rich oil drainage zone. Mechanical dispersion due to rock tortuosity and heterogeneities improved mixing of solvent with bitumen. In addition to these phenomena, relative permeability, capillary pressure, and heat transfer effects may also play a significant role. In order to obtain a better insight in the pore scale phenomena, micro-model experiment was carried out to gain further understanding. Three different solvents, toluene, pentane and propane are used in this study. The findings from this work significantly reduced the technical uncertainties, such as the level of asphaltene plugin in the matrix, the impact on fluid mobility, and ultimate oil residue which is directly linked to in-situ upgrading.

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Pore-scale modeling of acoustic events

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It is well established that acoustic emission is generated during hydraulic fracturing. Acoustic emission is used to find the volume effected by hydraulic fracturing, which is known as stimulated rock volume (SRV). Understanding the flow and transport properties of SRV is important as it effects the EUR of the oil reservoirs. In this study we analyze the change in permeability using pore scale modeling of the acoustic events.

We conducted a hydraulic fracturing experiment on a block of Tennessee sandstone in the lab and recorded the acoustic emission events generated during fracturing; the hypocenters of the acoustic emission are the positions where fracturing occurs. We then integrated the acoustic emission data into a physically representative pore-scale model of the sample developed based on petrophysical measurements. The pore-scale model is a regular lattice. We generate different realizations for the network model, with different numbers of acoustic events integrated into it to capture all the different acoustic events. We solve and upscale the model to predict the permeability change at the core scale.

We hypothesize that if the acoustic event density at any location in the sample block is below a certain threshold value, we can predict the change in transport properties, such as absolute permeability compared to intact conditions using the principles of the percolation theory. To test our hypothesis, we compare the predicted results with lab measurements. The permeability measurements (data) are obtained on core plugs that are extracted from the sample block after fracturing.

Our results indicate that in regions where the acoustic event density is below the threshold, there are only isolated fractures that are poorly connected, therefore there is no change in absolute permeability compared to intact conditions. But in sample region where this acoustic density is above the threshold value, there are enough fractures present for a percolation spanning cluster to occur. Hence, this region of the sample contains a macroscopic fracture that results in high permeability compared to the intact conditions.

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Syngas production from solid fuels using porous media combustion

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Filtration combustion is studied experimentally to examine the suitability of the concept for syngas production. In this work, the combustion of natural gas and air (lean mixtures) travel in a porous media reactor composed of ceramic foam and aleatory solid fuel particles (polyethylene and wood). In porous media reactor the solid fuel is heated and gasified under the gaseous products of the combustion of natural gas, as oxygen is expected to remain from the combustion of natural gas. Wood particles shows that accelerate polyethylene reactions. Flame temperature and wave velocity increased with an increase of polyethylene fraction in porous media reactor. The hydrogen and carbon monoxide were dominant products.

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An approximate Description of the Nonequilibrium Processes that Drive Incremental Oil Recovery in Carbonates at High Advancing Contact Angles

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Improved oil recovery from tight carbonate formations may provide the world with a major source of lower-rate power over several decades, but the mechanisms of incremental oil production have not yet been fully quantified. Here we will introduce a theory that tightly bounds the maximum advancing contact angle in spontaneous, piston-type water imbibition into mixed-wet rock, and will elucidate the dependence of this maximum contact angle on the highest capillary pressure in primary drainage of formation water by asphaltenic oil, receding contact angle, and shapes of pore cross-sections. The proposed model provides a conceptual framework for numerical simulators that will be able to predict incremental oil recovery in low permeability mixed-wet carbonates flooded with low(er) salinity brines. Currently this predictive capability does not exist. We will show that piston-type water imbibition is the main driving mechanism of incremental recovery, provided that the changed water chemistry lowers the advancing water contact angle below a critical value, which we establish from the modified Mayer-Stowe-Princen theory. Piston-type water imbibition can only happen when a three dimensional concave towards water Main Terminal Meniscus (MTM) proceeds into an oil-filled angular pore with water filaments along the pore corners. This happens either when the meniscus makes contact angle equal to advancing contact angle with the interior parts of the pore walls, or if it merges at zero contact angle with water swelling inside the pore corners and wall roughness. For advancing contact angles more than 90 deg on oil-wet surfaces, MTM is convex and thus cannot spontaneously imbibe.

Therefore, for an MTM to invade under a small but positive capillary pressure it must seamlessly merge with the corner water filaments. The MTM invasion is highly dynamic as it slides over the flat portions of the pore walls with a zero contact angle. We will explain in some detail how this happens.

We will use the published properties of micritic carbonates and other experimental data from literature to illustrate our model. There is substantial experimental evidence from corefloods and contact angle experiments from several labs supporting the proposed mechanisms of slow incremental recovery of asphaltenic oil in mixed-wet carbonates with high (>90 deg) advancing contact angles, but injection of a lower salinity seawater, sometimes diluted and with added new ionic species, is required.

This evidence comes in two flavors: (i) The low(er) salinity brines decrease advancing contact angle to allowable values predicted by the theory developed in this presentation; and (ii) The observed long tails (>10 injected pore volumes) of incremental oil recovery in low pressure gradient corefloods can be completely explained by the slow adjustment of a myriad of water/oil menisci to accommodate the spontaneous pore-by-pore piston-type imbibition of injected water, followed by cooperative pore-body filling and snap off.

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Contribution of electrical double layer repulsion to wettability alteration: from pore scale to molecular scale

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Waterflooding strategies by designing injected ions have been proved a promising enhanced oil recovery method in recent twenty years, including low salinity waterflooding (LSF) in sandstones, and seawater, low salinity water, or other designed water flooding in carbonates. Researchers generally believe that brine with designed ionic composition could alter the formation wettability to more water wet thus increase oil recovery. Various mechanisms have been proposed to explain such wettability alteration but no consensus has been reached. Electrical double layer (EDL) repulsion was one of the most frequently proposed wettability alteration mechanisms. Actually, EDL repulsion has been identified as one important crude oil-brine-rock interaction before the rise of waterflooding strategies by designing injected ions. In this paper, we aim to quantify the contribution of EDL repulsion to wettability alteration by both pore-scale continuum theory and molecular dynamics (MD) simulation. First, we integrate charge regulation EDL model with surface forces theory, and calculate contact angle variation due to change of salinity, saline ion valence, potential determining ions, and initial wettability. We find that: (1) the contact angle variation is restricted in 20 degrees due to EDL repulsion's contribution, (2) the optimum brine concentration for EDL repulsion is around 0.01 M-0.1 M and salinity effect of NaCl solution is more significant than that of CaCl2 solution, (3) the potential determining ions may bring more benefits at low total salinity, (4) the EDL repulsion may be more applicable to alter wettability for initially moderate water-wet systems. Since the continuum theory is more suitable for macroscopic drops and may not be good at describing microscopic interfacial phenomena, we use MD simulation to further study the contribution of EDL repulsion to wettability alteration. We clarify the deviation between continuum theory and MD results for nanodrops, and prove that pore size could influence wettability alteration in nanochannel. This paper tries to provide a systematic understanding of the relation between EDL repulsion and wettability alteration.

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Enhanced Oil Recovery by Low Salinity Water and Surfactant: Learnings from Coreflooding in Darcy and Micro Scales

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Low salinity water (LSW) flooding has been an attractive enhanced oil recovery (EOR) technique at which the incremental oil recovery is attained by manipulating the type and amount of salt in the injected water. LSW injection has been proved to have incremental oil recovery compared with conventional waterflooding. The underlying oil mobilization and recovery mechanism(s) has been under debate. The relatively unknown mechanisms are however believed to result in wetting change to a more water wet state especially in sandstone rocks. Another major advantage of LSW is the synergy it provides for chemical EOR at which high salinity is often a major challenge leading to less stability and high loss of chemicals. Therefore, injection of surfactant in low ionic strength brines where the ionic compositions were different has been the focus of this study. The low salinity surfactants (LSS) were injected after a LSW injection with exactly the same ionic composition. Therefore, there was also an opportunity to study the LSW injection. Subtle differences in the ionic composition of the injected LSS in 10cm-long aged Berea sandstone cores resulted in different residual oil saturations and end-point relative permeabilities. It was observed that the ionic composition which resulted in lower residual oil saturation depends on the aging duration before EOR injection. Since the interfacial tensions (IFT) at LSS solutions were not in the ultralow range (<0.001mN/m), it is discussed, based on the measured end-point relative permeabilities and IFTs, that wettability and its changes would be more important than IFT in LSS, compared with relatively higher importance of ultralow IFT in optimal salinity surfactant injection. The composition which resulted in lower residual oil saturation in LSS injection resulted also in stronger wetting change. In all experiments, before the LSS injection, the LSW was injected at both low and high injection rates. The equivalent velocities at low and high rate injections were 1.3 and 13 ft/day, respectively. Depending on the aging duration and ionic composition, systematic oscillations in the pressure drop profiles were observed after several pore volumes of LSW injection at low rate. The oscillations continued several hours and at some points were accompanied with oil recovery. This behavior showed that some compositions cause slower wetting change in LSW injection. The other part of this study was the coreflooding in a microcomputer tomography (micro-CT) machine to further investigate the pore scale phenomena in LSW and LSS injections with different ionic compositions. Configuration of residual oil clusters and their size distributions showed that in LSS injection the lower residual oil saturation accompanied with stronger wetting change. Lower residual oil saturation at stronger wetting change had also been observed in ordinary coreflooding. The core sample was initially strongly water wet. The change in wetting which provided mobilization of oil by LSS was from strongly water wet to (weakly) water wet. The small differences in ionic composition of injected LSWs affected also the residual oil saturations and its configuration. Moreover, it was also attempted to relate the wetting change behaviors to interfacial rheology.

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Experimental Investigation of the Performance of Carbonated (CO2-saturated) Low Salinity Brine Injection as a Novel EOR Scenario

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Water flooding (WF) is the most commonly used secondary oil recovery method; however, the average oil recovery by WF is very low; therefore, a significant amount of oil will remain in place after WF. To produce the trapped oil, different Enhanced Oil Recovery (EOR) scenarios have been developed. Two currently emerged water-based EOR scenarios are low salinity brine injection and carbonated (CO2-saturated) water injection (CWI). CWI can improve oil recovery through two major mechanisms that are fluid-fluid and rock-fluid mechanisms. The extents of these mechanisms are a function of the CO2 content of CW which is a direct function of the brine salinity and the saturation pressure of CW. At the same time, it has been shown that low salinity brine injection has the potential to favourably change the wettability state of the mixed-to-oil-wet sandstone reservoirs and therefore improve the oil recovery. Through the inclusion of CO2 in the low salinity brine or in another word merging CWI with low salinity brine injection, we can simultaneously take advantage of the oil recovery mechanisms of these water-based EOR scenarios. We called this novel EOR scenario as the carbonated low salinity brine (LSCW) injection.

In this study, we are aiming to investigate the potential of this new EOR method for improving oil recovery in oil-wet sandstone reservoirs. For this purpose, four core flood experiments have been performed on one type of Berea sandstone in which the potential of sea water, low salinity brine, carbonated water and LSCW injections as secondary injection scenarios have been investigated. The wettability of the cores was restored by ageing the rocks inside crude oil. The experiments were performed at a pressure and temperature of 2500 psi and 100 F. Moreover, to investigate possible wettability alteration by each method a series of contact angle measurements have been performed at a pressure and temperature of our coreflood experiments. To keep the consistency between our contact angle and coreflood experiments, same fluids and rock have been used.

The results of our coreflood experiments revealed that the inclusion of CO2 in low salinity brine can significantly enhance the performance of low salinity brine injection and at the same time it will help to better performance of CWI. Based on the flooding results, secondary low salinity brine injection and secondary CWI led to 3.3% and 11.1% OOIP additional oil recovery, respectively. However, secondary LSCW injection led to 15.8% OOIP additional oil recovery. Furthermore, the results of our wettability studies revealed the stronger potential of LSCW for changing the wettability state of oil-wet Berea rock toward more water-wet conditions compared to the low salinity brine. Based on our observations, low salinity brine could not change the wettability of the strongly oil-wet Berea rock, however, LSCW changed the wettability by 26 degrees toward more water-wet conditions. The difference between the extent of wettability alteration by LSCW and CW was negligible.

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Flooding of North Sea chalk and greensand cores with specific brines

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Four chalk and four greensand core samples from two oil-fields in the Danish North Sea were cleaned and restored to native oil saturation with dead oil and synthetic reservoir brine, before being aged and flooded with a sequence of brines with varying ion content. The purpose of the experiments was to observe any enhanced oil recovery (EOR) effects and to shed light on the mechanisms behind such effects. To further this purpose all samples were characterized petrophysically before and after testing and monitored by P-wave velocity and electric resistivity during aging and flooding. Effluents of oil were quantified by image analysis of photos for large quantities and radioactive tracer for small quantities (Katika et al. in press). Effluent brines were analysed by ICP-eos. In addition to the experimental work, numerical pore-scale flow and transport modelling as well as geochemical modelling were done. Aging and flooding were done at the relatively low temperature of 60oC in order to mimic reservoir temperature of the Gorm field. Each sample was flooded with a sequence of brines containing the same single cation (either Mg2+ or Na+) and varying combinations and concentrations of Cl- and SO42- followed by fresh water. The rationale was to test for: 1. The effect of salinity (as EOR effects were reported for sandstone by e.g. Seccombe et al. (2008); 2. The specific effect of the divalent Mg2+and SO42- ions (as EOR effects were predicted for chalk (although at higher temperature) by e.g. Austad et. al. (2008)). EOR effects were noticed for chalk when flooded with SO42- bearing and less significantly with Mg2+ bearing brine in spite of the low temperature of 60oC. Additional oil recovery was noticed, also in late stages of flooding. Pore scale modelling indicates that this can be caused by transport of oil in separate ganglia. EOR effects due to low salinity flooding were noticed neither in chalk nor in greensand. The chemical composition of the effluent brine changed in a piston manner reflecting the composition of the subsequent injected brines. At the same time the electrical monitoring indicated that only a part of the pore space was flooded in both chalk and greensand. Three EOR mechanisms were discussed: Wettability alteration, Fines formation, and Changes in pore compressibility. Wettability alteration was noticed in one case, where the originally water wet chalk became intermediate wet during aging as indicated by electrical data. No data indicate that return to water wetness gave rise to increased oil production. After flooding, all chalk samples behaved as water wet, whereas Nuclear Magnetic Resonance data indicate that all greensand samples remained mixed wet during the entire procedure. Fines formation,

probably due to precipitation of sulfate was observed in one chalk sample from shifting of the mercury injection curve to smaller pore throats. Geochemical modelling indicates that fines formation, followed by emulsification and increased viscosity can be a significant EOR mechanism. An increase in pore compressibility following flooding of chalk with Mg bearing brines cause a modest EOR effect.

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Is the pore volume (PV) injected in the lab scale equivalent to the PV injected in the field scale?

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In a coreflooding experiment in the laboratory typically a volume of water equivalent to several pore volumes (PV) of the porous rock, say 10 PVs, is injected in order to measure the oil recovery or residual oil saturation (Sor). In a field, 10PVs injection is not economically feasible, particularly when the process involves injection of costly chemicals (surfactant, polymer…) or designed water injection where the water composition is engineered. Although, this leaves a question mark, in terms of process costs in field scale, on how sound the lab experiment designs are, we continue to inject several PVs in the lab; and later on attempt to upscale the findings to the field scale and predict the possible outcome in the oil reservoirs. Therefore, it is necessary to determine either the designs of the lab experiments have to be revisited or to prove that the lab PV is not equivalent to the field PV. Or it is required to prove that obtaining Sor in the lab by injection of several PVs does not render the process economically ineffective in the field scale; in other words, not attaining Sor after injection of, say 0.2 PV in the lab, does not make the process less attractive in the field applications. Having assumptions of homogenous rock, incompressible fluids, 1-dimensional flow, constant and uniform velocity, piston-type displacement and no dispersion in the flooding front in an interwell system, a simple formulation was used in order to calculate how many PVs an imaginary core is receiving at different parts of the assumed reservoir. The formulation is started with only single-phase flow in a large reservoir and then generalized to a two-phase flow system where water displaces oil. The imaginary core was supposed to be at three different saturation zones of in front of flooding front (downstream), between the flooding front and the residual saturation front, and behind the residual oil saturation front (upstream). Different formulations were developed for different zones. The main result is that the volume the imaginary core receives behind or close to the residual saturation front is proportional to the distance the flooding front has from the injection well divided by the length of that core. The received water volume by the imaginary core depends also on the saturations, i.e. in an EOR process after waterflooding, where the oil saturation is already low (Sorw), the injected water volume will be even more. For example, depending on the well spacing (100s of meters), a 10cm-long core receives a water volume equivalent to 100s of PV of the imaginary core if it is located behind the residual oil saturation front or around it. The simple formulation in this work shows that a core sample depending on its position relative to the flooding front can receive a water volume equivalent to 100s of its PV. Therefore the injection of several PVs in the lab does not mean that the process would not be economic if performed in the field scale.

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Mathematical Models for Advanced Waterflooding: Oil Ganglia and Surface Chemistry of Carbonate Rocks

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Recent advances in oil recovery improvement using modified water injection require for the development of relevant mathematical models capable of explaining the observed trends. This work addresses the mechanisms of mobilization of residual oil and its flow in porous media, together with the estimation of the parameters to account for the surface chemistry of carbonate rocks. It is commonly accepted that after conventional flooding in the water-wet rocks the oil remains trapped in the swept zones in the form of disconnected oil drops, or oil ganglia. While the macroscopic theory of multiphase flow assumes that fluid phases flow in their own pore networks and do not influence each other, the flow of disconnected oil ganglia requires an alternative description. We address this problem by considering a micromodel for the two-phase flow in an angular pore-body. We find that presence of flowing water films on the surface of the rock can increase the velocity of the oil phase. Moreover, the flow of oil may be induced solely by the action of viscous forces at the oil-water interface, which appears to be a new mechanism for the transport of disconnected oil ganglia in porous media. We derive correlations for the calculation of phase flow velocities in pore bodies based on the pore fluid saturations. The macroscopic model, accounting for oil ganglia, is based on the assumption that active species in the injected brine cause the wettability alteration resulting in the formation of water films. Oil ganglia are mobilized and carried by the slow flow of wetting films. Considering simplistic pore-network model, we derive the macroscopic system of equations involving a description of the transport of oil ganglia. As a result of numerical modeling of the tertiary recovery process, it is found that production of oil ganglia may continue for a long time of injection of tens of PVI, similar to the production trends from the oil-wet rocks. Our simulations indicate that non-instantaneous wettability alteration may result in a considerable delay between the start of modified water injection and arrival of mobilized oil at the effluent. One of the possible chemical mechanisms through which the mobilization of the residual oil may occur in carbonates is an alteration of the electrostatic potential of the surface. Reduction of the surface charge due to adsorption of the potential determining ions: calcium, magnesium, and sulfate, - results in the decrease in oil affinity towards the surface of the rock. We analyze the data on the produced brine composition from the flow-through experiments [1] to estimate the parameters of the adsorption model. To investigate the effect of surface composition on the flooding efficiency, we combine the adsorption model with the Buckley-Leverett model and perform simulations of the experiments concerning flooding in a completely water-wet outcrop chalk [2]. Our computations demonstrate a correlation between the concentration of the adsorbed sulfate and the ultimate recovery, indicating that a more negatively charged surface of chalk could be a factor that affects the recovery efficiency without wettability modification.

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Modelling of Modified Salinity Waterflooding: A Comparison between the Mechanistic and Empirical Models

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Waterflooding is the most widely applied method of improved oil recovery. The majority of the studies show that lowering or modifying the salinity of the injected water seems to alter the wettability towards more water-wet conditions and increases the displacement efficiency of water-flooding. Analysing the porous media at sub-pore-scale shows that geochemical reactions occurring in the aqueous phase and at the crude oil/brine-mineral interfaces play an important role in changing the wettability, and consequently the relative permeability of the aqueous and oleic phases and the residual oil saturation to water-flooding. Different mechanistic and empirical models have been suggested to investigate the effect of modified-salinity water-flooding on the production history and the ultimate oil recovery. The mechanistic models include aqueous phase reactions, oil-water and rock-water interface reactions in the calculations, while the empirical models neglect the complex interaction between oil, brine and rock. Both group of models, however, estimate the transport properties of the oleic and aqueous phases by interpolating the relative permeability and capillary pressure curves between two different curves that are measured in extreme conditions, e.g., very high and very low salinities. Compared to the empirical models, the mechanistic models suffer from a computationally expensive reactive transport stage, while providing a more physical interpolation between the experimentally measured transport properties. In this study, we model a large set of core flooding experiments on the Stevns Klint chalk samples using empirical models and compare the results with an in-house mechanistic model in terms of the computational time and accuracy of the models. We first obtain the relative permeability parameters by fitting (history-matching) a two-phase flow model to the reported core flooding recovery data in different formation brine and injection brine compositions, temperatures, pressures, and oil compositions. For the empirical group of models, we assume that salt is transported as a pseudo-component in the aqueous phase with/without adsorption on the rock, and we assume that the relative permeabilities are a function of the total salinity. In the mechanistic model, we solve a reactive transport model that considers the aqueous and surface complexation of ionic species and the dissolution/precipitation of the minerals. We finally compare the performance of the models for different experimental conditions.

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Pore scale reactive modelling of dynamic wettability alteration

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We present a pore scale model capable of simulating two-phase flow with ionic adsorption at the fluid/solid interface. We use Direct Numerical Simulation of the Navier-Stokes equations to simulate the flow. The phase distribution is solved using the Volume-Of-Fluid method. The transport of chemical species is given by an Advection-Diffusion-Reaction Equation with an additional flux at the fluid/fluid interface resulting from the jump of concentration. In this work, we assume that the change of wettability observed during low salinity flooding in carbonate rocks is related to the change of surface charge, induced by the adsorptions of potential determining ions, such as calcium, magnesium or sulphate, onto the rock surface. This is modelled using surface complexation modelling with Langmuir adsorption isotherm. We then assume for simplicity that the contact angle changes linearly with the surface potential. The model is applied to study wettability change in a 2 by 2 square pore network. We discuss the differences in the flow pattern for various initial conditions and maximum contact angle change. We observe that the dynamic change in wettability can lead to invasion of the four pores if the adsorption of ions precedes the water front, i.e. when the diffusion is large enough and the retardation related to the adsorption is small. This gives us new insights into the importance of flow patterns for low salinity effect and is consistent with experimental observation of higher oil recovery due to more pores being invaded during low salinity flooding.

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Pore scale simulation of electro-chemical induced wettability changes in three dimensional pore scale geometries

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The oil recovery process in a given reservoir depends on the mineral composition and the chemical constituents of the brine and the reservoir oil. The electrochemical exchange processes between the mineral surface and the water, and between the oil and water interface, are a central processes for EOR applications with injected water. Our approach is to simulate the wettability change by modeling the interfacial and surface processes that control the corresponding surface energies.

Brines with a controlled chemical composition have the effect of altering the mineral surface in terms of dissolution and precipitation of mineral compounds. We use a pore scale lattice Boltzmann model to account for these effects [1]. This model has been extended to account for two fluid phases, and it includes a model for coupling the aqueous chemistry with the surface energy of a given mineral, so that the wetting properties of oil and water, and the associated capillary forces, can be accounted for. We have used the Chan-Mitchell model [2] for the surface energy between the water and the mineral, and adapted this model to the lattice-Boltzmann framework.

The surface energy is a function of the equilibrium concentrations of the species in the aqueous phase (or electrolyte), and we can then study the wetting alterations that are caused by altering the chemical composition of the injected water, including low salinity water.

In the current work we present a model for the wetting properties based on the electrochemical interaction between the aqueous phase and mineral wall. In general, the presence of ions in the water corresponds to the buildup of surface charges and an electric double layer in the aqueous electrolyte. It is well known that this double layer formation corresponds to a lowering of the surface energy, and the maximum surface energy is obtained for a neutral surface (”point of zero charge” (PZC)) [3-5]. Hence, it is energetically favorable to expand the area of this low-energy charged surface, and the surface becomes more water wetting, with a reduced contact area between an oil droplets and the surface.

Results from simulation on realistic 3D pore geometries will be presented together with analysis of the restriction on up-scaling using the pore scale simulations.

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Reservoir fluid composition and the implications for modified salinity flooding

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The research presented here forms part of an ambitious, targeted effort to improve recovery of oil and gas from the Danish North Sea chalk fields. For all enhanced oil recovery applications, the composition of the water phase of the reservoir fluid is crucial. The original formation water in the reservoirs varies significantly in salinity; however it is typically 2-3 times the salinity of sea water. In addition to sodium Na+ and chloride Cl- the most important ions generally observed in the formation water are Ca2+, Mg2+, K+, SO42-, Ba2+, Sr2+. The main difference between the formation water and the seawater apart from total salinity, is that seawater typically contains 3-6 times more sulphate than formation water and no significant amount of barium and strontium. The effect of ionic strength of the aqueous phase in the reservoir on the propensity of petroleum to adhere to chalk is not fully understood, but it has been shown experimentally that lowering the salinity of the injection water has a positive effect on oil recovery under certain circumstances. This is known as low salinity water flooding and one of the goal is to investigate this effect in chalk and to discover the optimum salinity of the injection water.1 Experiments on carbonate rocks have also shown that changing the concentrations of ions in the injection water, including SO42- and Mg2+, has a positive effect on oil recovery under certain conditions. This is one of the recovery mechanisms known as SmartWater. The effect of additional sulphate on the reservoir fluid is subject to debate, but a hypothesis is that the sulphate affects interactions between positively charged sites on the chalk surface and polar compounds in the oil. The ion bridges may help release the polar compounds from the rock and increase oil mobility. Magnesium is known to exchange with calcium on the rock surface and studying the extent of this exchange is one of the points of interest in this project. A thorough analysis and characterization of the reservoir fluids, including the petroleum fluids and the formation brine, is required for optimizing these techniques and understanding the underlying chemical mechanisms. The ionic composition of injection water and the composition of the polar compounds in the oil have wider implications for rock surface chemistry studies, corrosion studies, core flooding experiments, and reservoir simulation and modelling.

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The link between crude oil – brine – rock interactions and low salinity EOR in sandstone reservoir systems

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Laboratory research and field pilots have shown that a low salinity (LS) brine can be used as an injection brine to enhance oil recovery in sandstone reservoirs. An average recovery increase of 14% beyond ordinary water injection has been reported from laboratory tests, and in 2017 BP is commencing low salinity water injection in the Clair Ridge field, offshore UK. Why low salinity brine injection work so well in increasing oil recovery, is still under debate, but there is a general consensus that the increased oil recovery is a result of wettability alteration of the rock surface to a more water-wet state. To improve oil recovery by wettability alteration to a more water-wet state requires that the initial wetting is less water-wet, i.e. mixed-wet, which is not always the case. A mixed wetting in a rock is a result of a combination of chemical interactions between the three complex phases; crude oil, rock and brine. The crude oil contains polar organic compounds that are the molecules, which anchors the oil phase to the rock, and create a wetting. However, the crude oil components are not able to wet the surface at all conditions. There are conditions where sandstone reservoirs behave water-wet, even though there is crude oil present in the reservoir. The ability of the crude oil components to wet the surface is dependent on the rock-brine interactions, and especially on the resulting pH in the reservoir. When the water entered the rock millions of years ago, chemical reactions took place between the water and the rock minerals. Depending on the type of minerals present, the chemical interactions varied, but an equilibrium pH was created in the pore water. When oil invaded the reservoir, chemical reactions, controlled by pH, allowed the oil to wet the surface, or not. In water-based EOR processes in mixed –wet reservoirs, the challenge is to reverse the process, and be able to remove the crude oil anchor molecules in a wettability alteration process. A chemical mechanism has been proposed for the wettability alteration process taking place during the injection of low salinity brine. The wettability alteration process is initiated by rock-brine interactions as the low salinity brine is injected, followed by crude oil – brine – rock (COBR) interactions that release the crude oil, and result in enhanced oil recovery. In this paper, the circumstances where a rock can become mixed-wet or water-wet are explained by crude oil – brine – rock interactions. Preferable conditions for observing low salinity EOR effects are demonstrated. Finally, an unfavorable COBR system showing no LS EOR effects is manipulated to become favorable, showing positive LS EOR effects.

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Wetting dependent relative permeability and its effect on oil recovery

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Description: Some experimental data suggest that low-salinity water injection leads to more water-wet behavior and "consequently" to improved oil recovery. Based on the sketched behavior in the paper by Lomeland, Ebeltoft and Thomas (LET), we derive LET relative permeability curves that only depend on irreducible water saturation. High irreducible water saturation is both indicative of pore size heterogeneity and water-wet behavior. Admittedly this is a gross oversimplification but gives the relative permeability behavior in terms of one parameter as opposed to seven. We use the theory of Buckley-Leverett to construct recovery curves for 1D and 2D displacement and various mobility (M = displacing fluid mobility / displaced fluid mobility) ratios. We solve the equations in 1D and 2D both analytically and numerically (Chen, Hopmans and Grismer, COMinisymposium OL 5.2©). The simulations show that water-wet behavior is conducive to stable displacement and high recovery at breakthrough, whereas oil-wet behavior is conducive to high ultimate recoveries.

Application: Investigation of the effect of wettability on the recovery behavior

Results, Observation, Conclusion: • Wettability has a significant effect on the recovery efficiency. • High irreducible water saturation is both indicative of pore size heterogeneity and water-wet behavior. • At high mobility ratios the displacement efficiency, i.e. the recovery at breakthrough is less. However, a low end point permeability, which occurs for strong water-wet behavior leads to a lower mobility ratio and hence to more stable behavior. • The simulations show indeed, that water-wet behavior is conducive to stable displacement and high recovery at breakthrough, whereas intermediate-wet behavior is conducive to high ultimate recoveries. • It is possible to use a method suggested by Hopmans et al. in COMinisymposium OL to perform 2-D Buckley-Leverett simulations

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Zeta potential in oil-water-carbonate systems and its impact on oil recovery during controlled salinity waterflooding

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We use an integrated experimental method to demonstrate that improved oil recovery (IOR) during controlled salinuty waterflooding (CSW) is strongly correlated to changes in zeta potential at both the mineral-water and oil-water interfaces. We report experiments in which IOR during CSW occurs only when the change in brine composition induces a repulsive electrostatic force between the oil-brine and mineral-brine interfaces.

IOR is observed with decreasing salinity in conventional Low Salinity Waterflooding (LSW) but also increasing salinity in inverted LSW so long as the change in zeta potential induces a repulsive electrostatic force between the interfaces. IOR is also observed for waterflooding at constant ionic strength so long as selective changes in ion concentration yield similar changes in zeta potential.

Results also show that the zeta potential at the oil-water interface may be positive at conditions relevant to carbonate reservoirs. A key challenge for any model of CSW is to explain why IOR is not always observed. Here we suggest that failures using the conventional (dilution) approach to CSW may have been caused by a positively charged oil-water interface that had not been identified.

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A MULTISCALE MODEL FOR WATER AND NUTRIENT UPTAKE BY PLANT ROOTS : FROM SINGLE ROOT TO ROOT SYSTEM SCALE

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Aims: Water and nutrient transfer to plant roots is a multiscale problem determined by processes within the µm to the m scale. A spatially distributed continuum mechanistic description of these processes would require a sub mm discretization with high computational demand for an entire full grown root system that extends over the meter scale. .

Methods: A coupled multiscale model for water and nutrient uptake from a single root to the root system scale has been developed . We used the 1-D radially axisymmetric model of Barber and Cushman (1981) to describe nutrient transport to a single root segment. Transport to the entire root system is represented by a network of connected cylindrical models around the roots. This network of cylinders was coupled to a 3-D regular grid that was used to solve the flow and transport equations Flemisch et al. (2011) in the soil at the root system scale.

Results: Cumulative nutrient uptake simulated by the coupled multiscale model compared well with the approximate analytical solution of Roose et al. (2001) and with simulations using a spatially highly resolved 3-D mesh while reducing computational costs.

Conclusions: The multiscale coupling approach allows simulating water and nutrient transport at the root system scale with minimal computational cost and good accuracy. This approach also accounts for the effect of root architecture and soil conditions (e.g. water content) on nutrient uptake.

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Coupled root water and solute uptake – a functional structural model

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Understanding the distribution and fate of solutes in the soil-plant continuum is of interest for regulatory authorities, customers and producers. For example pesticide legislation requires numerous modelling and experimental studies to exclude environmental risks before a substance receives authorization. The standard modelling approach used in these procedures, however, does not hold detailed information about the fate of the solute in the plant root system, but treats the root system as a linear sink term. Uptake is determined as fraction of the mass flow which is given by the transpiration multiplied with the soil liquid concentration . With the increasing availability of more detailed modelling approaches within the last years, we focus on a more mechanistic description of pesticide uptake by plant roots. R-SWMinisymposium is a three dimensional model for water movement in soil and plant roots [1]. It also includes solute transport within the roots, which is realized as a particle tracking algorithm [2]. We coupled this model to Partrace, another particle tracking algorithm that solves the convection-dispersion-equation in the soil. Active or passive solute transport across the root membrane is included in the model. While active transport, namely Michaelis-Menten kinetics, requires energy input from the plant, passive transport can be either driven by advective water uptake and/or by the local concentration gradient between root and soil. Root membrane conductance is determined by the lipophilic properties of the solute. Within the root system solutes are transported via the advective water flux. We further implemented microbial degradation of the substance and sorption to both soil and roots. Benchmarking the coupled 3D model with an analytical solution for a single root at steady state flow conditions showed good agreement. Using this new approach we could derive global uptake parameters in silico and compare the simulation results to data from hydroponic plant uptake experiments. The detailed modelling approach enables tracking solutes in time, space and phase within the soil and root system. This novel simulation tool can be used to investigate the influence of soil properties, root system architectures, solute properties, meteorological conditions as well as plant management strategies on plant solute uptake to gain a deeper understanding of solute uptake and transport parameters.

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Hybrid Mixture Theory Based Modeling, and X-Ray Micro-CT based Validation of Unsaturated Transport and Microstructural Changes in Foods During Frying

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Hybrid mixture theory was used to derive unsaturated transport and thermomechanical stress equations for a viscoelastic biopolymeric matrix. The two-scale laws of conservation of mass, momentum, energy and entropy were utilized, the constitutive theory was formulated, and the entropy inequality was exploited to obtain various equilibrium, near-equilibrium and non-equilibrium relations. The system was treated as poroviscoelastic with the viscoelastic biopolymers interacting with the viscous water and oil phases at pore-scale via hydrophilic and hydrophobic forces. Exploitation of the entropy inequality resulted in non-Darcian integro-differential law of fluid flow, near-equilibrium swelling and capillary pressure relations, generalized stress relations, near-equilibrium Gibbs free energy relation and the rate of evaporation relation. The generalized Darcy's law relation includes an integral term with long-memory effects. This can describe the effect of time-dependent polymer relaxation on both Darcian and non-Darcian modes of fluid transport depending upon the state of the biopolymers (glassy, rubbery or glass-transition). The unsaturated generalized Darcy's law relations were validated by making comparisons to the experimental data on moisture transport, heat penetration and pressure development during frying of potatoes and chicken nuggets. The solution was obtained by transforming the transport equations from Eulerian to Lagrangian coordinates. Interesting observations about unsaturated transport mechanisms, the role of gas and pore pressure and texture development in foods were made. Validation of mechanisms was performed using image analysis of micro-CT images and by performing lab experiments. Micro-CT images also showed that a crispy layer was observed slightly underneath the surface, which is counter-intuitive. The same was predicted by the model. The results were used to make conclusions about modifying the frying process for obtaining healthier foods with reduced fat uptake.

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Metastatic growth processes within brain tissue

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Research on the hallmarks of cancer, cf. [1], is mostly based on in-vivo and in-vitro experiments. Therein, characteristics of metastatic processes are observed on different scales. Whereas in-silicio, multi-scale cancer modelling can transfer results from in-vitro cancer-cell experiments to the macroscale. This contribution demonstrates the use of in-vitro cancer cell growth and atrophy experiments for computational studies of continuum-mechanical models. Additionally, the results are compared to a computational benchmark study, cf. [2].

The metastatic processes of interest are lung cancer growth and atrophy within the brain tissue. In the initial step, cancer cells may pass the blood-brain barrier (extravasation) and invade the surrounding tissue. In the following, a sufficient nutrient supply triggers the formation of micrometastases originated from the cancer cells. Furthermore, the cancer cells stimulate blood-vessel sprouting leading to large interveined metastases. This crucially affects the tissue in terms of induced stress, disruption of the cells and creation of leaky blood vessels. A promising option to treat the metastases and its consequences is to infuse a therapeutic agent into the extravascular space of the brain tissue close to the metastasis site. The introduced processes are described in a continuum-mechanical model in the framework of the Theory of Porous Media (TPM), cf. [3]. This macroscopic multi-phasic modelling approach is based on a volumetric homogenisation of the microscopic structure over a representative elementary volume. Consequently, superimposed and interacting continua of the constituents are achieved. In particular, the constituents are an elastic solid skeleton (brain cells and metastases) and two immiscible pore liquids (interstitial fluid and blood). Moreover, the pore liquids are itselves real mixtures of miscible components. In particular, the components of the blood are the solvent and the cancer cells, which may extravasate into the solvent of the interstitial fluid. In addition, the interstitial fluid contains nutrients and a therapeutic agent. The metastatic processes of atrophy, growth, extravasation and angiogenesis are described by mass exchange terms. In particular, the nutrient-dependent cancer cells can either proliferate or elsewise undergo starvation (necrosis). Besides necrosis, the pressurised infusion of a therapeutic agent into the interstitial fluid causes the death of the metastases (apoptosis). Furthermore, the parameters for atrophy and growth can be derived from in-vitro cancer cell experiments.

The model is governed by the overall momentum balance and the adapted mass balances relations. Therefore, the primary variables are the solid deformation, the liquids' pore pressures and the concentrations of the solved components, cf. [4]. Numerically, the partial differential equations are solved monolithically, applying the inhouse finite-element package PANDAS. The discretisation in space is carried out by extended Taylor-Hood elements. Furthermore, the model is discretised in time by an implicit Euler time-integration scheme. Finally, numerical examples are compared to a benchmark study not only to demonstrate the feasibility but also to outline the different modelling approaches and advances of the introduced model.

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Microporous Changes in Frozen Foods Subjected to Freeze-Thaw Cycles

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Freezing is one of the most important methods to extend the shelf life of foods. However, the damage to frozen products may occur due to temperature fluctuations during storage and shipping. Freeze-thaw cycles may cause textural changes, moisture migration and ice recrystallization in the frozen materials. The objective of this study was to investigate the effect of temperature fluctuations on ice crystals growth/decay in the frozen potatoes, using X-ray micro-computed tomography (CT). Microporous characterization is an important quality parameter in foods. By analyzing the imaging results, the microstructural properties, such as porosity and pore size distribution were obtained, which are needed for modeling transport phenomena during freeze-thaw cycles and for designing/optimizing the freezing process. Potatoes with cuboid French fry shapes were frozen at -80 °C (control group) and fluctuated between -17 to -16 °C, -17 to -11 °C and -17 to -7 °C for one and two weeks duration. X-ray micro-computed tomography (CT) was used to observe 3-dimensional (3D) microstructure of frozen potatoes. The series of micro-CT images were rendered into 3D structures by performing image analysis. Segmentation and pore size analysis were conducted to obtain pore size distribution and ice crystal growth/decay information. Image analysis showed a significant growth of ice crystals with the increase in temperature fluctuations and the duration of freezing. Conversely, the total number of pores reduced with increase in amplitude and time duration of freeze-thaw cycles. At the temperature fluctuation between -17 and -7 °C, there were only 1,275 and 851 pores left in the samples when compared to 10,549 in the control group. In addition, the pore size distribution clearly became broader as the temperature fluctuation and freezing time increased, which shifted the range toward 10 mm3 when the sample was frozen between -17 to 7 °C for two weeks. These results demonstrate that the micro-CT and image analysis can be used to analyze the microstructure of frozen materials and obtain valuable information for designing the freezing process.

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Mixed-dimensional models for flow, transport and growth processes in porous media with embedded biological network systems

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Models of root water uptake and nutrient uptake in crops and soil evaporation processes can help to understand plant water management during an agricultural season. For newly planted crop seeds root growth processes are equally important for the water management. Models of competing crops growing in close proximity to each can help understanding if such processes are influenced by the competition for water or nutrients.

The large number of roots demand dimensionally reduced models of the network systems to describe the interaction with the surrounding bulk soil on a plant scale. We present a mixed-dimensional method featuring two coupled PDE systems, one posed on a three-dimensional bulk domain, the other posed on a one-dimensional network domain that is geometrically embedded in three-dimensional space. Similar methods for root water uptake have been developed in e.g. [1,2]. However, particularly in systems with growing networks, issues of both mass conservation and scale separation have not yet been addressed. We suggest a locally mass conservative scheme including growing root networks. The consistent coupled framework allows for growth algorithms strongly coupled with soil properties and quantities like porosity, water saturation, nutrient concentrations. We employ a growth algorithm developed by [3,4] and extend it with a dependency on soil quantities.

Very similar processes occur in a different biological system. Mathematical models of flow and transport processes in and between the blood microcirculation and the surrounding extra-vascular tissue can contribute to understanding complex biological processes and guide treatment of vascular diseases and cancer. The microcirculation features ongoing adaption and auto-regulation processes altering the geometry. Tumor at a certain size, induce angiogenesis -- capillary growth -- in order to increase oxygen and nutrient proliferation. Embedded mixed-dimension methods for tissue perfusion have also been investigated in literature [5]. They present an improvement over methods where micro-scale quantities are volume-averaged and upscaled yielding homogenized model descriptions on the macro-scale. Instead of upscaling certain interesting features, as the capillary network geometry in a vascularized biological tissue, network features are discretely resolved. The model could help bridging scales between microcirculation and organ scale cardiovascular models.

For both applications we developed locally mass-conservative finite volume coupling schemes in a framework flexible with respect to the models employed in each sub-domain.

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Modelling heat and mass transport in frost-resistant plant tissues under frost exposure

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Plant tissues have developed several strategies to cope with temperatures below the freezing point. Some of these strategies are of physiological nature, others arise from structural properties. Here, the focus is in particular on the structural properties of plant tissues. A key mechanism is the dehydration of the cell body, as freezing within the cells is a critical process, which threatens the structural integrity and even the ability of a plant to survive. Another important mechanism is the controlled flow management capability, which is mainly determined by structural properties of the cell bodies. Thus, the water leaves the cell body and flows within the vascular bundles to preferred locations, where freezing is not assumed to be critical [1]. The aim of this contribution is to assess this behaviour by a multicomponent and multiphasic model within the framework of the Theory of Porous Media (TPM) [2].

Frost-resistant plant tissues can be understood as a porous material, as they are formed by cells with prescribed intra- and extracellular spaces. A sound continuum-mechanical model can be realised within the TPM, where processes on the microscale can be related to a homogenised macroscopic model. This is achieved by a volumetric homogenisation of the microscopic structure within a representative elementary volume (REV), resulting in superimposed and interacting constituents. According to [3], frost-resistant plant tissues are described by considering four constituents. The model proceeds from a thermoelastic and isotropic solid skeleton, which is formed by the cell bodies, which contain initially trapped water. Within the pore space two mobile fluids are present, namely, materially compressible air and materially incompressible water, where the latter can be subjected to a phase transition and turns into ice, which is then kinematically coupled to the solid skeleton. The interaction of the constituents can be described by so-called production terms in the balance equations of mass, linear momentum and energy.

The key mechanisms that are considered within the continuum-mechanical model are consequently the cell dehydration, the flow management capability of the plant tissue and the freezing process of the pore water. The first mentioned property is taken into account by a production term in the mass balance of the solid skeleton (and the pore water), where the water is with decreasing temperature no longer trapped within the cell body. The flow management capability can be described by anisotropic permeability conditions. The freezing of the pore water is characterised by a jump in density at the interface and the coexistence of both phases during the freezing process. The interface is conceptionally treated by a singular surface, at which a mass transfer can be formulated with the help of jump conditions according to [4]. The resulting system of coupled partial differential equations is solved numerically using the in-house developed Finite-Element (FE) code PANDAS. The numerical examples illustrate the behaviour of frost-resistant plant tissues and show in particular the anisotropic perfusion and the freezing of the accumulated cell water at preferred locations.

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Moisture-driven cellular deformation in thick- versus thin-walled cell plant systems

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We consider two cellular model systems subjected to changes in moisture content: softwood (spruce) tissue in presence or absence of sap and fruit tissue (apple). Using X-ray micro-CT (computed tomography) imaging (both laboratory and synchroton-based), we document the geometric changes of the materials during moisture content variations. The three-dimensional investigation of wood and fruit tissues tomographic datasets during moisture-induced deformations (swelling/shrinkage) at cellular and sub-cellular scales highlights the effect of the different cell wall structures. Such studies are needed e.g. in the engineering of the drying process of cellular materials. X-ray tomography is used to unveil the wood and apple tissue microstructures at different stages of dehydration. Different image analysis procedures are required to identify deformations at the cellular scale [Patera et al. 2016]. The morphological analysis uses an automated characterization protocol [Herremans et al. 2015] to identify individual fruit cells and void space network. The cell size, cell anisotropy, cell wall thickness, porosity and void connectivity variations are also recorded during dehydration. Softwood tissue consists mostly of longitudinal tracheid cells and of radially oriented ray cells, the latter representing 5% of the wood volume. Across the growth ring, the thin-walled earlywood cells with large internal lumens change to thick-walled latewood cells with small-sized lumens, thus with cell wall ranging from one to eight micrometers and cell lumens ranging from a few to 100's of micrometers. The wood cell wall is composed of four layers, of which the thickest wall layer, namely S2, is mainly driving the swelling behavior. We found an anisotropy in cellular hygrodeformation attributable to the alignment of earlywood cells and to the overall presence of rays. We document the collapse of thinniest earlywood cells during drying of sap, although most wood cells do not deform during sap drying. Fruit cellular structure consists of the cell protoplasm filling the cell membrane, which is bounded by the cell wall. The cell wall is in the few micrometers range and cell membrane in the 100-200 nanometers. Fruit cells can be considered filled with water-carbohydrate solution and are under turgor pressure at high water potential. Fruit is a soft cellular material that undergoes microstructural changes during dehydration, including large deformations, cell membrane breakage and cell wall collapse. These changes have a significant impact on its macroscopic properties, e.g. permeability. We document the sequential collapse of fruit cells at the air/fruit interface leading to the build-up of a dense drying layer, while the inner most section of fruit tissue undergoes little moisture content or deformation variations. The swelling/shrinkage behavior of multilayer cell walls is modeled using poromechanical upscaling from microscopic mechanical models and is used to investigate deformation of cellular wood and fruit tissues. This allows understanding the roles of aspect ratio, thickness of cell walls, layered system, etc. In the simulation, the cellular structure is adjusted according to the corresponding dehydration, and thus deformation, stage, resulting in an effective moisture permeability which has a strong moisture content dependency.

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Multi-scale characterization of diffusion phenomenon at the interface of cartilage and bone

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INTRODUCTION: Osteoarthritis (OA) is a disease affecting articulating joints and is associated with articular cartilage deterioration as well as alterations in the subchondral bone plate morphology [1]. Earlier studies suggested that in early stage of OA, subchondral bone alterations even precede cartilage damage [2]. Here, we investigate whether the interface of cartilage and subchondral bone is permeable to small molecules and to relate the diffusion process to the morphological features of subchondral bone plate and articular cartilage using combination of micro-computed tomography (micro-CT) and Focused ion beam-scanning electron microscopy (FIB/SEM). This study provides a platform for understanding the molecular exchange at the interface of cartilage and bone and how it may be affected by micro-architecture of the interface.

METHODS: Osteochondral plugs were harvested fresh from an equine joint (n=5, phi=8.5 mm). To study the diffusion from cartilage to subchondral bone plate, 500 µL of a neutral contrast agent (Iodixanol, MW=1550.2 g/mol) solution was placed on the surface of articular cartilage, while the lateral diffusion was prevented. Using a micro-CT (voxel size=20 µm3, Quantum FX, Perkin Elmer, USA), we monitored diffusion in a region of interest (ROI) containing cartilage and subchondral bone plate in various time points until 72 hours after adding contrast agent. The thickness and porosity of subchondral plate were calculated by local median thresholding (FIJI and BoneJ plugin). The average grey values at the subchondral bone plate post subtraction of t0 image at each time point were calculated. FIB cross sections were made with 30 kV, 0.3 nA and SEM imaging in BSE mode is done at 2 kV with the Through the Lens Detector in combination with the immersion lens.

RESULTS: Multi-regression analyses on equine samples revealed importance of cartilage thickness (p-value=0.019) and porosity (p-value=0.0011) and thickness (p-value=0.003) of subchondral bone plate on diffusion across the interface. The subchondral bone plate thickness was 269.1±128.9 µm and the subchondral bone plate porosity was 5.96±4.09 (%) and cartilage thickness was 1282±512.6 µm (Figure 1A). There was a strong correlation between the equilibrium grey value (near-equilibrium diffusion) and porosity of subchondral bone plate (Figure 1B). The FIB/SEM picture of the subchondral bone plate also revealed that majority of the pore size was between 10 to 30 nm (Figure 2).

DISCUSSION: Early OA is associated with thinning of subchondral bone plate and increased plate porosity [3, 4]. Nevertheless, thickening and densification of subchondral bone plate is the hallmark of later stages of OA [5]. Studying solute diffusion at the interface of cartilage and subchondral bone could provide information on its dependence on the morphological characteristics of subchondral bone plate and cartilage in different stages of OA. Our findings depicted strong linear correlation between diffusion and porosity, suggesting that inter-connected pores at the interface of cartilage and subchondral bone plate could facilitate solute transport. Our data revealed that diffusion of molecules up to

~1.5 kDa could occur at the bone-cartilage interface. Beside micro-CT, we will adopt FIB/SEM imaging to perform multi-scale approach on the solute transport across cartilage and bone.

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Numerical analysis of second order elliptic problems with small inclusions

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Many geological and biological systems, like fractured shale rock layers, vascularized tissue or soil containing root networks, can be considered as porous media with small inclusions. In order to reduce the computational effort for simulating flow in complex inclusions, dimensional reduced flow models, in particular one-dimensional (1D) flow models are used. However, the coupling of 1D PDEs with three-dimensional (3D) PDEs governing the diffusive flow in the surrounding porous matrix is not trivial, since one has to bridge a high dimensional gap between the different models. A possible way to couple 1D and 3D flow models is to formulate in a first step suitable source terms which account for the mass transfer between the inclusions and the porous medium. In a second step, the 1D model is embedded into the 3D domain by inserting Dirac measures into the source term of the 3D model, where the Dirac measures are concentrated on the surface of the inclusions or on the main axes of the inclusions. The objective of this talk is to analyze this way of coupling by means of a second order elliptic model problem. In particular, model reduction errors, the regularity of the solution and the convergence behavior of standard finite elements are studied. The theoretical results obtained by this analysis are confirmed by numerical tests.

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Observations on preconditioning the 3d-1d coupled problems

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We consider a model problem where two elliptic PDEs posed on domains with different dimensionality are coupled through a trace constraint enforced by means of Lagrange multiplier. In \cite{2d-1d} efficient preconditioners for the case where the dimensional gap between the domains is one were established based on the properties of the continuous trace operator and operator preconditioing \cite{precond}. In particular, the problem was proved well-posed with the Lagrange multiplier in the dual space of $H^{1/2}$ and the preconditioner used the corresponding Riesz map whose discrete approximation utilized the spectral decomposition of Laplacian. Our current contribution discusses the case where the dimensionality gap is two, specifically, the lower dimensional domain is a curve embedded in the three dimensional domain. In this setting the continuous trace operator is not well defined unless higher regularity assumptions are used or the solution is sought in non-standard spaces, for instance weighted Sobolev spaces \cite{dangelo}. However, the functions in H^1 conforming finite element spaces are continuous and the trace makes sense. Therefore we focus on the discrete problem and mirroring \cite{2d-1d} the preconditioner shall be constructed as a suitable power of the Laplacian. Using series of numerical experiments we demonstrate that such a construction leads to a good preconditioner for the model problem. It is also shown that if the relevant inf-sup like condition is respected the discretization of the two domains can be independent. In particular, the elements of the curve are allowed to cross those of the three dimensional domain.

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The Effects of Microporosity on Thermoregulation and Ventilation in Termites's Mounds from Pore-scale simulation in Micro-CT Images

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Mounds of termites have long been studied as fascinating examples of thermoregulation of animal buildings due to their built-in temperature-buffering property, permitting stable mound temperatures throughout the year. This property may be driven by the interplay of: metabolism, evaporative cooling, passive diffusion, or external flow. There is however very little information in literatures on the role of pore structures—both macro-, and micro-structures—in accommodating thermoregulation and gas exchange.

The closed-ventilation system of Trinervitermes Geminatus mound relies on passive diffusion for aeration. Little is known about how precisely the micro, and macrostructure of the mounds drive such mechanism. First, for our macroscale model, we obtained X-ray images of Trinervitermes geminatus mounds from Guinea and Senegal with millimetre resolutions using medical X-ray scanner. Then, for our microscale model, we took a fraction of each samples and obtain micron-resolution images using X-ray Micro-CT scanning. Direct numerical simulations of flow and diffusion within the microscale pore spaces give us flow fields, fluid permeabilities, tortuosities and formation factors of these structures. Subsequently heat transfer simulations within the grain spaces give the effective heat conductivity of the mounds' microstructure.

From flow simulations, we found that the permeability of the Guinea sample is smaller than the Senegal, whereas the flow is more tortuous in the former compared to the latter. From diffusion simulations, we can compute the formation factors of the microporous structure of the mounds; we found that the fluids in the Senegal sample have three-times larger effective diffusivity coefficient than in the Guinea counterpart. For the next step, we input effective diffusivity and heat conductivity from the microscale simulations into our macroscale transport models which are computed on pore and grain spaces of our millimetre-scale images. We are able to simulate gas exchange and heat transfer between the core and the exterior wall of the mounds under realistic conditions, which include diurnal heating of the walls.

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A Spectral Element Model for Detailed Heat Flow in Shallow Geothermal Systems

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This contribution introduces a new analytical model capable of simulating fully transient conductive-convective heat transfer processes in a shallow geothermal system consisting of a borehole heat exchanger embedded in a multilayer soil mass. The spectral element method is utilized. The proposed model combines the exactness of the analytical methods with an important extent of generality in describing the geometry and boundary conditions of the numerical methods. It calculates the temperature distribution in all involved borehole heat exchanger components and the surrounding soil mass using the discrete Fourier transform, for the time domain, and the modified Bessel functions, for the spatial domain. Numerical examples illustrating the model capabilities for simulating transient heat transfer in a shallow geothermal system subjected to short and long term time varying boundary conditions will be presented. The CPU time for calculating temperature distributions in all involved components; pipe-in, pipe-out, grout, and soil is only few seconds in an Intel PC.

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An approach for simulation of hydraulic stimulation of a fractured geothermal reservoir

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Stimulation of fractures in igneous and metamorphic rocks can enhance the permeability of critically oriented fractures with orders of magnitude at pressures elevated below the minimum principal stress. Complex THMC couplings dominate the subsurface processes. A numerical approach for modelling of shear dilation of fracture networks in a three-dimensional low-permeable matrix is developed, focusing on the hydro-mechanical coupling. The approach is based on a conceptual discrete fracture-matrix (DFM) model where the dominating fractures are modelled explicitly and surrounded by low-permeable matrix, capturing the effect of small-scale fractures on the flow. The rock matrix is assumed linearly elastic, while a fracture deformation model handles the frictional shear-slip and dilation of the fractures, coupled to the matrix by internal boundary conditions. Applying recently developed finite volume-type discretizations, simulation results can be obtained for three-dimensional test cases (e.g., as shown in Figure 1 for a simplified fracture network geometry) to investigate stimulation scenarios. In particular, the DFM model makes it possible to study the effect of matrix permeability on the hydraulic stimulation of the fracture network.

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Critical temperature of permeability change in thermally cracked granite

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The permeability of Luhui granite with 200mm in diameter by 400mm long was measured at triaxial stresses and elevated temperature by “600℃20MN servo-controlled triaxial rock mechanics testing machine”. It is found that 300℃ is the critical temperature (Tc) of permeability change with temperature in thermally cracked granite. The magnitude of permeability is 10-7 Darcy with a low increase below Tc and the permeability whose magnitude is 10-6Darcy increases drastically with high amplitude at 300℃-400℃ while the magnitude is 10-5Darcy at 400℃. Simultaneously, the change of micro-crack quantity in thermally cracked Luhui granite at temperature up to 400℃ was quantificationally investigated by MPV-SP micro-photometer. Two peaks of micro-crack quantity that the length is more than 5μm and 10μm respectively exist at temperature up to 400℃. The temperature scope of micro-crack quantity peak in length>5μm are less than that in length>10μm. The quantity of micro crack whose length is more than 10μm increases sharply at the rate of one per ten degree at temperature above 300℃. The drastic increase of micro crack above 300℃ is the main reason that permeability increases sharply at temperature above 300℃ in thermally cracked granite.

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Downhole Thermoelectric Power Generation System in Geothermal Well

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Geothermal energy is a clean, renewable energy resource that is widely available and reliable in the world. It's regarded as an effective way to meet the challenge of deteriorating global climate and environment. Power generation is one of important utilizations of geothermal. The traditional geothermal power generation needs to extract geo-fluid to surface and reinject the cold water into formation. Practice and literature survey show that this practice has many problems such as wellbore scale, formation blockage, microquakes or subsidence and others. In this study, a novel downhole thermoelectric power generation system in geothermal well is presented. A thermosiphon heat exchanger, a downhole cold water circulation loop with a number of thermoelectric cells is proposed for this research. The thermosiphon heat exchanger transfers heat from deep hot reservoir to upper cold reservoir along the wellbore and forms the hot side of thermoelectric power generation. The downhole cold water circulation loop inner the wellbore circulates the cold water from surface to downhole and forms the cold side of thermoelectric power generation. The thermoelectric cells locate between the thermosiphon heat exchanger and the cold water circulation loop. They generate electricity when a temperature difference is created due to Seebeck effect. The thermal models are developed and the power generations are analyzed. The overall thermal-to-electricity efficiency of the proposed system is up to 7-9%. Comparing with traditional geothermal power generation system, the proposed system has advantages of less capital cost, minimum ground space, absence of wellbore and formation scale, and microquakes or subsidence risk free. It's a promising way to develop and utilize geothermal energy.

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Enhanced geothermal systems using chaotic advection

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Enhanced geothermal systems recover heat from underground reservoirs employing a static pair of injector-producer wells. However, heat recovery in this static configuration may be suboptimal due to inefficient distribution of production fluid throughout the reservoir. Such traditional geothermal systems admit first modeling by a 2D Darcy flow in a circular reservoir driven by a source-sink pair located diametrically opposite to each other along the circumference. Recent studies in literature [1,2] have shown that through systematic reorientation of the source-sink pair, the so-called rotated potential mixing (RPM) flow, may become capable of accomplishing chaotic advection. This can in practice be implemented in the field by having a static array of wells, separated by an angle theta, placed along the circumference of the domain. The effect of reorientation of source-sink pair can then be achieved by periodically turning off the current operating pair and turning on the pair located theta apart. Chaotic advection can in principle boost performance by distributing production fluid throughout the reservoir domain which can dramatically enhance heat recovery. However, the studies [1,2] consider isotropic conditions, whereas realistic reservoirs are anisotropic.

We theoretically and computationally investigate the (chaotic) advection of production fluids in both isotropic and anisotropic systems. The numerical analysis centers on a dynamical-systems approach making use of so-called Poincaré sections to visualize the transport of the production fluid. Such Poincaré sections enable identification of regions of chaos and coherent structures in RPM flow for different anisotropic configurations and pumping protocols. This facilitates systematic investigation of the impact of anisotropy on transport characteristics. Poincaré sections for isotropic media reveal several symmetry curves (red, blue, green) as shown in Fig 1, with visible island structures which form transport barriers limiting mixing and scalar transport. Introducing anisotropy changes the picture drastically, with the placement of the wells relative to the permeability direction playing a critical role. Anisotropy generically eliminates key organizing mechanisms in the Lagrangian transport, viz. symmetries, and thus tends to promote disorder and, inherently, chaotic advection as shown in Fig 2. However, symmetries are partially preserved and thus order and coherence partially restored in non-generic cases such as pumping schemes employing an even number of injector-producer wells with well configurations aligned with the anisotropy direction as demonstrated in Fig 3.

We further rigorously examine the link between fluid distribution and heat transfer in RPM flows with the ultimate goal of designing effective pumping schemes for optimal heat recovery. The evolution of temperature fields obtained under different reservoir conditions is compared with Lagrangian transport characteristics and analyzed to quantify production efficiency of EGeneral Session s for different well configurations and pumping schemes.

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Experimental research of seepage law of fractured granite under high temperature and high pressure

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By using high temperature and high pressure triaxial permeability facilities, the seepage law of fractured granite under different temperature and pressure was studied. By analyzing the permeability evolution with temperature and pressure, the deformation and crack characteristics of granite under different temperature, different pressure and different pore pressure was revealed, and the re-crack formation of fractured granite under high temperature and pressure and its influence on seepage law are obtained. The results are very useful in HDR geothermal exploitation

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Geothermal Systems Performance Assessment and Environmental Impacts

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Problems associated with fossil fuel consumption has increased worldwide interest in discovering and developing sustainable sources of energy. One such system is geothermal heating which uses the constant temperature of the ground to heat or cool buildings. In recent years, the popularity of geothermal heating has increased due to its reliability, convenience, and accessibility and it is expected that in the near future, most large buildings will have geothermal pumps as part of their heating/cooling system. Geothermal heating systems can use ground source heat pumps (General Session HPs) to circulate a fluid that is cooled or heated through the subsurface. These systems are usually installed in the upper few hundred feet of the earth's surface where temperature changes with atmospheric conditions are minimal so they can use the stable temperatures as a heat battery to heat and cool homes, schools, and businesses. During the winter, heat is pumped from the subsurface into buildings; in the summer, it is transferred from the structure into the ground by reversing the process. Today, General Session HP systems are one of the fastest growing applications of renewable energy in the world, with most of this growth happening in the USA and Europe. In the present research, the performance and environmental impacts of a vertical closed-loop General Session HP system is evaluated, using typical Canadian climates. To do so, the required thermal load of an office building in three different Canadian cities is calculated. The cities are selected based on their temperature norms and their heating/cooling runtime which results in various ground heat loads. Using a three-dimensional model, developed using FEFLOW, groundwater flow and heat transport is simulated in the geological formation where the Borehole Heat Exchanger (BHE) field is installed. The model demonstrates the effects of geothermal heating on subsurface in terms of temperature plumes and thermally affected zones. Furthermore, a thorough sensitivity analysis is conducted to determine the sensitivity of the model to parameters like groundwater flow, building thermal load, BHE configuration and BHE properties. The aim of this study is to provide an understanding of the performance of General Session HP systems in different climatic zones in Canada along with the environmental impacts of long-term use of these systems. This research will ultimately help better regulate geothermal systems to make ensure high efficiency while limiting their environmental impacts.

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Online-experiment investigation of permeability ore-bearing rock under the stress-temperature and the evolution pore-fissure in microscopic structure

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Hot dry rock geothermal energy development, oil and gas resources in oil shale in situ thermal production, in situ dehydration and modified property of lignite resource, and nuclear waste geological disposal, geological sequestration of CO2, shale oil and gas, natural gas hydrate exploration is widely energy and resources exploitation engineering. Must study the pore-crack evolution of ore-bearing rock, under the effect of seepage, stress, temperature, chemical, namely the evolution of the porous medium, synchronization online measurement of permeability coefficient should be carried out under the stress and temperature evolution. Taiyuan university of technology development of a THMC coupling testing machine with the 200-600 ℃ high temperature， and online measure permeability of granite, oil shale, coal, and the evolution of the pore- fissure by microscopic CT, the experiment and conclusion respectively described as follows: 1) During the thermal cracking of granite at 200℃, very few small cracks are observed. When the temperature increases to 300℃, some small cracks coalesce into bigger fractures, the lengths of which increase by approximately 10 times. Mylonitic grain structures are presented in the granite specimen at 500℃. More than 90% of the thermal cracking fractures are along the relatively weak cement faces which are around the rock particles.The thermal cracking process of granite is characterized by intermittence and multi-stages. From room temperature to 600℃, two severe cracking periods exist. The permeability of granite presents several peaks along with the appearances of the cracking periods. The granite permeability presents several peak value stages and they lag behind the peak value stages of the AE parameter E. Overall, the permeability of granite increases with the accumulation of the AE peak value stages. 2) We studied the evolution of lignite pore microstructures by micro-CT, From room temperature to 600°C, pore-structure evolution of lignite occurred in three phases. At room temperature to 200°C (phase I), the numbers of pores and fissures, and the specific surface area increased rapidly. At the end of this phase, the porosity increased to 37.9%, the percolation probability exceeds the percolation threshold of 31.17% and seepage begins. During phase II (200°C–500°C), pyrolysis increased the numbers of new pores and fissures significantly. The original and newly developed pores and fissures become interconnected to form larger pores and pore groups. The specific surface area and porosity increased slowly. During phase III, from 500°C to 600°C, the porosity increased rapidly to 47.8%. 3) oil Shale deposit is huge reserves, and undeveloped important unconventional oil and gas resources, Authors devotes to the in situ thermal oil shale mining research for more than 20 years. Under the action of different distillation temperature, by micro-CT technology for study pore and microcracks of oil shale, expounds the change of microscopic pore and fracture, provides scientific guidance to thermal exploitation in situ of oil shale.

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Reservoir Modeling of a CO2 Plume Geothermal System

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Previous research has proven the general potential of C02-based geothermal energy systems (CPG) coupled with either continuous carbon dioxide sequestration or making use of a finite amount of C02. For the first time, we focus on the experimental design of a C02-limited CPG system using topographical information. We investigate the feasibility of CPG for the test site with emphasis put on absolute distance and elevation difference between the wells and establish a general link to the present topography. We prove that the topographical gradients are not steep enough to focus the migration path of the carbon dioxide plume towards the production well. Additionally, we show that the performance of the CPG system decreases with decreasing vertical permeability.

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A multi-scale approach for numerical modelling of the subsurface CO2 sequestration process.

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Subsurface carbon dioxide (CO2) sequestration is a promising technology to reduce CO2 emissions into the atmosphere. After injection, the carbon dioxide plume can migrate until it is fully trapped. Four major mechanisms play an important role in trapping which include structural trapping, residual trapping, dissolution trapping or mineralization. The accurate numerical simulation of the sequestration process is challenging owing to the complexity of buoyancy driven enhanced dissolution and convective propagation of the CO2 plume. To resolve these processes, one often needs an extremely fine computational grid which makes the CPU time prohibitive for modelling at reservoir scale. Several simplified models were proposed which include analytical models [1], vertical equilibrium models [2,3] and a multi-scale application of dissolution rate models [4]. Here we applied and extended the multi-scale application for modelling of CO2 sequestration on the large-scale. Several numerical experiments are considered using adjusted small-scale simulation of the plume dynamic in a sloped aquifer. The enhanced rate of dissolution captured in the small-scale models with geometrical properties was then applied to the simulation in the realistic aquifer. A sink term applied to the CO2-brine-interface is implemented in the ADGPRS program. This term numerically acts as the dissolution mass transfer that would otherwise occur in a compositional simulation at fine resolution. It is important to contemplate the slow reduction in dissolution rate after the fingers begin to interact with the bottom of the reservoir. After interaction becomes significant a reduction in the local dissolution rate is considered. We compared our multi-scale approach with a high-fidelity compositional simulation at high resolution similar to the results presented in [5]. The applicability of the proposed approach was validated on the numerical model of a realistic aquifer.

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Adapted models for the study of thermal effects of CO2 injection at different spatio-temporal scales

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The simulation of CO2 injection and migration into a geological formation is a computational problem that can be considered several temporal and spatial scales. While the study of a specific injection operation may range from years to decades and involve a CO2 plume extending a few kilometers from the injection well, the subsequent migration of CO2 may last for centuries or millennia and involve migration distances of hundreds of kilometers.

When studying the introduction of large amounts of CO2 in an aquifer, understanding thermal developments is important. Temperature has a significant impact on fluid densities and viscosities, geomechanical stresses, phase mixing and rates of geochemical reactions. The injection of CO2 at considerably lower temperatures than the storage site itself has been proposed for technical and economic reasons [1]. As a different example, the study of natural analogs may also involve hot CO2 intruding into a geological formation at a significantly lower temperature [2].

The inclusion of thermal modeling in a flow simulation incurs significant computational cost. If other effects, such as geomechanics, have to be taken into account, the computational problem grows larger still. For this reason, it becomes desirable to employ simplified models whenever appropriate.

A range of models of different complexities can be used to model thermal development. At one extreme, a full 3D multi-phase simulation including the energy conservation equations for each phase and leakage of heat into the overburden will in some cases be necessary. However, in other situations simpler models may be warranted, including models based on vertical equilibrium [3, 4], one-phase models to compute heat convection, and even analytical models for simplified geometries. The rate of heat convection versus heat conduction will determine the extent to which heat leakage needs to be modeled. The choice of most suitable model will depend on several factors, in particular the temporal and spatial scales under consideration.

In this study, we investigate the ability of different models to adequately represent thermal developments in a CO2 storage setting, in particular in terms of spatio-temporal scales, with the goal to identify the simplest suitable model for a given circumstance. To this end, we have implemented simulations models of different complexity using the MATLAB Reservoir Simulation Toolbox [5] and its CO2lab module [6]. This includes a vertical equilibrium model for CO2 flow that includes heat leakage out of the formation based on a complete model of diffusion into the overburden.

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Experiment and model on the CO2 exsolution from oil in microporous

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The performance and mechanisms of CO2 enhanced oil recovery (EOR) have been investigated widely during passed decades. However, for some complicated CO2 EOR strategies proposed in recent years, i.e. huff and puff process or CO2-steam coupled process, the better understanding on the mechanisms in pore-scale are necessary. Other than the CO2-oil-water interaction under constant reservoir pressure and temperature, during the huff and puff or steam coupled CO2 EOR process, the reservoir pressure and temperature change significantly. These reservoir condition change, will consequently result in the miscibility and solubility change of CO2-oil-water system. In study, a microporous visualization experimental system which can provide a variable pressure (in range of ambient pressure to 15 MPa) and temperature (in range of room temperature to 80 oC) is set up and the CO2 exsolution from oil in microporous due to the depressurization or heating induced solubility reduction has been investigated experimentally. We also explore the influence of depressurization rate and heat flux on the nucleation and growth of CO2 during the exsolution process. With higher depressurization rate and higher heat flux, there is more CO2 nucleation and the size of single bubble is inclined to be smaller. The quantitative pressure and temperature dependency of the exsolved CO2 volume and mass for the depressurization and heating process are obtained based on the pore-scale images. The behavior of CO2 exsolution in microporous from the aqueous phase is also investigated for comparison with light oil and the results show significant difference, indicating strong dependence of the exsolution process on the solvent fluid properties. We also compare the observed phenomenon to a pore-scale gas exsolution model, and modify the model to fit the case of CO2 exsolution from oil in microporous better.

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Forecasting the migration of a buoyant fluid using spill-point analysis, with application to uncertainty quantification of CO2 storage capacity in structural traps

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To mitigate climate change and reduce greenhouse gas emissions, permanent storage of CO2 in geological formations is considered a promising strategy. Commercial and demonstration projects around the world have already been capturing CO2 from point sources and injecting it into saline aquifers for long-term storage or for research purposes. The geological formations selected ideally have a caprock that the buoyant CO2 cannot permeate, and thus it will become confined to a thin layer under the sloping caprock or be trapped inside structural “domes” as it continues to migrate upwards and over large lateral distances. This so-called structural trapping is one of the first trapping mechanisms likely to take place after injecting CO2. As such, the identification of structural traps and their capacity to contain the buoyant CO2 can provide useful information when deciding on the location and rate of injection wells.

In this work, structural traps are identified through a spill-point analysis on the top surfaces of various formations. Based on the outcome of this analysis, a migration forecasting algorithm is used to predict the ultimate position of injected CO2, including how much CO2 will remain trapped within structural domes, and how much will flow out across the formation boundaries (assuming fluid exchange between the aquifer and surrounding aquifer systems is able to occur). The use of this forecasting algorithm reduces the need to simulate long-term migration of CO2, which is particularly advantageous when many simulations and/or realizations of a flow model are required for the purpose of optimization, uncertainty quantification, model calibration, etc.

In particular, this work demonstrates a workflow of how one could quantify the uncertainty of the structural trapping capacity associated with the top-surface of a formation. Since the lateral migration of CO2 depends highly on the shape of the caprock, the precise elevation and undulations of the caprock will dictate the trapping capacity found within its structural features. By using the migration forecast algorithm, the impact of geometrical uncertainty on trapping capacity and migration pathway can be evaluated without performing any numerical simulation of CO2 flow and transport, which means many realizations of the top-surface can be assessed within a reasonable time frame.

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Model comparison for geomechanical simulation of large-scale CO2 storage

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Large-scale CO2 storage will involve high-volume injection into deep saline aquifers lasting over several decades. CO2 injection must be carried out in a safe and economically feasible manner, ensuring that the geomechanical integrity of the seal, or caprock, is maintained at all times. Protection of caprock integrity requires a maintaining an allowable overpressure in the storage aquifer, which is the maximum value that can be sustained before fractures are created or activated in the seal. Fractures may lead to unwanted fluid leakage or unacceptable levels of seismicity, which can result in costly operational issues such as well shut-in, recompletion or abandonment of the project. The geological setting and geomechanical properties of the storage complex, as well as the volume and rate of CO2 injection, all contribute to the risks related to caprock integrity.

Deformations in the caprock are linked to pressure dynamics in the reservoir and the existing stress states prior to injection. It is essential to employ the most appropriate simulation tools that capture the temporal and spatial variation of relevant process that impact mechanical behavior and leakage of CO2 storage systems. The state-of-art approach to hydromechanical modeling is the coupling of two-phase flow of CO2 and and geomechanics, either by combining separate simulators or by a fully integrated code. In certain cases, it may be important to have two-way coupling to consider the effect of flow on geomechanics and vice versa. The creation or activation of fractures can occur due to shear and bending stresses from overpressurization, particularly within the damage zone around an existing fault. These impacts create significant risk of leakage, but the dynamics occur at a scale too small to resolve in large-scale models. Upscaling and simplification of sub-grid dynamics will be required, as well as new techniques to couple flow, mechanics and other physics or even chemistry at the reservoir scale.

Benchmark studies are valuable tools for understanding the impact of uncertainties on predictions for migration and storage security, but very little has been done for geomechanical problems related to CO2 storage. We propose an integrated geomechanics benchmark study to investigate relevant scenarios for caprock integrity—e.g. understanding acceptable reservoir pressure, modeling leakage scenarios, and concurrent injection operations. Realistic aquifer geometries and parameters are used from the Norwegian CO2 Storage Atlases to ensure the relevance of the problems for offshore CO2 storage. In making a comparison of simulation tools from each of the participating partners, we explore how different model approaches and couplings lead to different predictions, which give important insights for the modeling community and potential users.

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Reactive Transport Modelling of Geological CO2 Sequestration in Deccan Volcanic Province

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Carbon dioxide concentration buildup in earth atmosphere has been the major environmental concern as reported by Mauna Loa Observatory -current atmosphere CO2 growth rate is 2.11ppm per year [1]. CO2 geological sequestration is one possible technology for mitigating CO2 from being indefinitely emitted to the earth atmosphere. Authorities, universities and industry around the worldwide are investigating the feasible options for CO2 geo-sequestration. As of recent statistics availbale - India is having third position in CO2 emission[2]. In the United Nations Framework Convention on Climate Change (UNFCCC) Paris summit, India pledges 33-35% cut in carbon emission intensity by 2030 [2]. Inorder to achieve this, India need to explore novel CO2 mitigation options like CO2 sequestration. In India, Geological formations like Deccan Volcanic Province are promising option for carbon dioxide sequestration. Injecting carbon dioxide, normally in a supercritical state, into carefully selected hydrocarbon or saline formations gives rise to several physical, chemical and thermo-hydro-mechanical processes occurring at the reservoir and the surrounding region. Certain priliminary experimental studies regarding the sequestration capacity of Deccan volcanic province is investigated by Prasad et al (2009, 2012) [3, 4]. In this paper geological reactive transport modeling of Deccan trap formations is done with mineralogy and geochemical data from experiments conducted by Prasad et al (2009, 2012) [3, 4]. The reactive transport model is generated with the help of massively parallel reactive transport code PFLOTRAN on a desktop cluster. Inorder to improve parallel performance of PFLOTRAN in the desktop cluster OpenMPI is used as the message passing interface and Network File System (NFS) is used for the sharing of data between paralell processor cores. The main objective of the simulation is to understand the behaviour of deccan trap towards mineral trapping of CO2, which is the only permanent mitigation option available for sequestration. From the analysis of modeling results, the mineralization capacity of carbon dioxide sequestration is identified. But as time progresses there is a decrease in the pH of the formation because of the dissolution of Ca and Mg minerals, which are prominent in Deccan trap. As a result of the reduction in formation pH sequestration capacity of the formation starts to reduce. From the above observation, it can be concluded that short term CO2 sequestration projects at multiple locations of deccan trap are suitable for Deccan volcanic province other than a single long term sequestration project. Because for a long term project - the rate of change in pH should be less inorder to have almost uniform CO2 mineralization rate [5], else the resultant pressure buildup in formations may effect formation stability with consequences of CO2 leakage.

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A new meshless method for pore scale modeling of real rocks scanned by micro-CT

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Numerical simulation can be an efficient tool to understand real porous samples at pore scale. For this purpose, the involved methods have to be built considering the complexity of these geometries. In this talk we will expose some results aiming performing high resolution simulations, in order to investigate the inner nature of real world rocks.

The geometries used in our studies are obtained by micro-CT: this technique allows to voxelize the domain and to reuse it for the purpose of numerical simulation. In our work, the scanned data is treated to know the rock matrix by the use of a characteristic function, which takes advantage of the binary type data given by tomography. An algorithm has also been developed to identify the percolating connected components of the domain where fluid flows. Firstly, identifying the connected components guarantees the well-posedness of the Stokes problem, which can suffer from incompatibility condition in case of several connected components, even with global zero-flux and divergence-free velocity. Secondly, it prevents from performing any needless calculation and optimizes the simulation.

Aiming the modeling of inner flow inside rocks, we will present a new method based on a penalization and diffusion splitting. Penalization methods have widely and successfully been used for external flow computation and flow control. Within the proposed method, the whole solid part is penalized. The flow is calculated by the help of velocity/vorticity formulation, and the values are known on the data grid. As penalization, vortex methods are efficient for flow control, and additionally they are particularly suited for high resolution simulations. The use of vorticity field is also crucial for the completion of slipping or non-slipping conditions at the physical interface between rock matrix and fluid domain. The process is part of a grid-particle method, in which the velocity field is first computed on a fixed grid, solving Stokes equations. The obtained velocity is then used to transport a quantity (for instance, a mass concentration) inside the domain. The quantity is carried by particles, whose move is independent from the grid frame. The evaluation of velocity on these particles is made through a quadrature formula based on a measure solution.

The method is used on several geometries, such as Bentheimer rocks or beads network, which are both scanned from real samples. The obtained results are a way to check the robustness of the method in the context of geological real data. As a perspective and due to its robustness, this high resolution solver would be adapted to solve reactive coupling. The evaluation of porosity and permeability constants could also be one of the applications of the method, as a statistical treatment of flow rate on several simulations could allow to estimate these physical constants.

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Cavitation-driven crystallization pressure and back-fracturing of the growing salt

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Two ingredients are essential to build a crystallization pressure event in porous medium, supersaturation of the in-pore solution and persistence of a nanometric liquid film in-between the growing salt and the host crystal. The former supersaturation fixes the stress level attainable during the rapid growth of the precipitated salt. The latter film enables the rapid growth of the salt that enhances the disjoining pressure which is instrumental to exert stress on the close solids. Desarnaud et al. (2016) clarified that the stress force associated to crystallization pressure is indeed originating in the disjoining pressure. We developed drying experiments in silica rectangular capillary (200x20 µm) filled in with slightly undersaturated sodium sulfate solution. In a first step, thenardite crystals precipitated at the two liquid-air interfaces at both extremities of the tube, seemingly closing the tube. Actually, as demonstrated elsewhere (Bouzid et al., 2011; Hulin and Mercury, this conference), annular capillary menisci separated the salt caps from the capillary tube, giving rise to a capillary state in the film along the caps and behind. Most of the solution trapped in the tube was therefore under superheating state, what had been evidenced two years later when this solution cavitated. The superheated/capillary state is thermodynamically characterised by specific properties leading liquid water to be, in general, a better solvent than in its 'normal' counterpart. As a result, capillary water-solid interactions drives the solution to a larger concentration: the equilibrium constant gets a higher value. Thus, the cavitation of a superheated equilibrated solution (lifetime: two years) thermodynamically correspond to the transition of a saturated to a supersaturated situation at constant composition: only the equilibrium constant decreases brutally. In the experiment introduced above, the cavitation of a bubble in the superheated macrovolume was rapidly followed by a second event: the large fracturing of one of the thenardite caps. It can only be interpreted as the back-fracturing of the salt brutally growing due to the supersaturation spike, consequently enhancing the disjoining repulsive pressure in between the host and the guest solids. This higher value of disjoining pressure puts the two close solids under stress until the the most fragile broke out. This fracturing step was followed by a third step, a healing long period (9 months), during which fissures were sealed by reprecipitation of salt linked to the dissipation of the supersaturation. This last step has been completely overlooked in the classic studies about the rock damage by crystallization pressure, and could be a self-healing strategy whenever the damage remains limited.

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Impact of matrix deformations on drying of granular materials

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When granular materials such as soil or cement dry, large capillary pressures that develop along the air-liquid interface can deform the solid matrix by displacing particles. The mutual feedback between particle displacement, pore opening and capillary air invasion leads to the creation of highly preferential invasion pathways, which dry out faster while the remainder of the medium remains wet. Such heterogeneous drying maintains high drying rates leading to faster breakthrough as it sustains liquid connectivity to wet pores evaporating at the outer surface. We present here a pore-scale model which couples liquid evaporation, vapor diffusion, capillary air invasion and granular mechanics to study the impact of the initial microstructure on the drying rate and patterns. Our simulations show that preferential invasion prevails in more homogeneous media (narrower particle size distribution), since small changes in pore sizes and hence in invasion thresholds dominate over the initial disorder.

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A NEW MECHANISTIC MODEL TO PREDICT THE IMPACT OF BIOFILMinisymposium ON POROUS MEDIA HYDRAULIC PROPERTIES

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The accumulation of biofilms has significant implications for the design and management of a number of technological applications. The complexity of the microbial communities growing in porous media is not properly understood and it often implies a simplification in the modeling procedure. This highlights the need for a sound understanding of the components, structure and hydraulic characteristics of the microbial community, as well as of its spatial distribution. This work tries to bring some light on them, providing a new mechanistic model that predicts the variably saturated hydraulic properties of bio-amended porous media. Special emphasis is laid on the mechanisms of biofilm-affected soils to retain and let water flow through, providing valuable insights into phenomena behind bioclogging.

Our approach consists in modeling the porous media as an ensemble of capillary tubes of different diameters, obtained from the experimental biofilm-free water retention curve. This methodology is extended by the incorporation of a biofilm composed of bacterial cells and extracellular polymeric substances (EPS). Such a microbial consortium displays a channeled geometry that shrinks/swells with suction changes. The overall impact of biofilms can then derived by assuming that biomass reshapes the pore space following specific geometrical patterns. As a result, a new set of analytical equations for the volumetric water content and the relative permeability is obtained.

The model is discussed and corroborated by using data from laboratory studies and other approaches from the literature. Results show that it can reproduce i) displacements of the soil-water retention curve towards higher saturations and ii) permeability reductions of distinct orders of magnitude. From our findings, we are even able to explain how very small amounts of biofilm may fully reshape the pore network leading to significant changes in the hydraulic properties. Finally, we state the importance of accounting for the hydraulic characteristics of biofilms and for a complex/more realistic geometry of its bodies at the pore-scale.

9th International Conference on Porous Media & Annual Meeting, Rotterdam 2017, Submission 726

Bacterial accumulation behind a grain

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Flow surrounding an obstacle constitutes one of the classical problems on hydrodynamic, and it represents a basic model to understand flow in porous media. In this work, we generate a potential flow around a cylinder in a Hele-Shaw-like system (i.e. small distance between the upper and lower wall) by the use of microfluidics. Under these conditions, we report experimental evidence of accumulation of motile \emph{Escericha coli} behind an obstacle. We show that such accumulation - not observed with dead bacteria - depends on the imposed flow velocity. The flow simulation in this type of system suggests that areas with low flow velocity and low shear rates favorite the accumulation of bacteria. We also extended this work studying the effect of an obstacle's row lined up in the center of the channel.

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Bacterial accumulation in throttled flows

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In confined environments, such as narrow passages or porous media, bacteria suspensions can undergo significant modification of their transport properties. Under these conditions, both accumulations caused by ratchet arrangement, and attachment to surfaces leading to biofilm formation can be observed. In addition, the combination of flow and surface shape can have significant impacts on the microorganisms' behavior that allow processes such as rheotaxis to occur. Under these conditions, the transport of the bacterial suspension differs significantly from passive suspensions. Here we systematically test this scenario on Escherichia coli suspensions flowing in a straight channel with a funnel-like constriction in the middle[1]. This constriction is characterized by the aperture (Wf) and its angle (Θf). We explore how the modification of Wf and Θf affects the accumulation of bacteria in the channel. Concentrations of bacteria passing the constriction were observed for all the cases. However, the range of flow rates producing such accumulation varied with the geometry. We are able to partially reproduce the experimental results using a simple phenomenological model containing the different forces experienced by E. coli in a confined geometry[2].

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Bacterial dispersion in porous media

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Dispersion of particles in porous media is a classical problem well studied where physical laws are well established.

Recently, observations of motile bacteria in a flow revealed that shear orients the body of the bacteria and influences their trajectories. This coupling designated by the term of rheotaxis has been mainly studied at the particle scale or in simple Poiseuille flow, we here studied its influence on the transport in a porous media. For this purpose, we developed a specific microfluidic chip (aperture 100 microns) containing circular obstacles (diameter ranging between 10 and 150 microns) randomly placed between the top and bottom walls.

Thanks to the transparency of the chip, we tracked hundreds of trajectories of motile and non motile E coli bacteria and studied the influence of the flow velocity on their statistic. For flow velocity of the order of the bacterial mean swimming velocity, the analysis of the trajectories revealed that the motility reduce the longitudinal dispersion. In the same time, the transverse dispersion is enhanced. We will discuss these effects on the large scale transport of bacteria.

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Microbial dispersion in Confined & Heterogeneous Flows

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Within the shallow subsurface, soil, rock, fluids, gases and living organisms are in close interactions as a result of the coupling between flows, mixing, solutes availability and microorganisms displacement and adaptation. The common challenge in all these processes is their spatial variability (heterogeneity); the complexity rising from their coupling implies that predictions based on rates measured under homogenized, well-mixed, conditions may differ by orders of magnitudes from observations in the field. Recent studies greatly improved our current understanding of non trivial characteristics of microorganisms-flow interaction, such as microbial motility and the response to chemical gradients or microbial attachment to surfaces and the ability to form biofilm structures. My research focuses on the coupling between non uniform flows and transport of biotic and abiotic components of the subsurface, using microfluidics devices and time-lapse video-microscopy.

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The impact of flow on microbial evolution in porous environments

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Microbes are primarily studied in either liquid culture or on Petri dishes. However, these assays are a far cry from where bacteria really live. The overwhelming majority of bacteria live in porous environments, like soil, aquifers, and sediments, where they facilitate many important processes. Despite this, we understand little about how these complex environments shape the composition of the microbial communities that live within them. Here we address the complexity of these environments by combining microfluidic experiments with models of biofilm formation and fluid dynamics. We bring together concepts from number of historically disparate fields to show that canonical models of microbial competition do not necessarily hold in the environment in which most bacteria live. This also reveals that living in pore spaces fundamentally changes how bacteria evolve. We show that bacteria in porous environments face a fundamental dilemma: they rely on flow for nutrients and dispersal, however, as cells grow, they tend to reduce their access to flow, diverting it instead to competitors. Our results suggest that cells within a biofilms can obtain a competitive advantage by growing more slowly.

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X-ray CT-technology revealing the effects of denitrifying bacteria on porous limestone

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Paracoccus denitrificans has been used to study the effects of microbiologically induced nitrogen gas production and calcium carbonate precipitation within two porous limestones: Savonnières (France) and Tabaire (Spain). Both limestones are used as building materials and consist of a different pore network and therefore induce different fluid flow behavior. Primarily, the bacteria in suspension were flushed through the samples (i.e. colloid transport, e.g. Molnar et al., 2015) and counted with a flow cytometer to see if and how they got retained within the pore network. Additionally, the immersed limestone samples got stored at 36 °C and were imaged multiple times using X-ray Computed Tomography (X-ray CT) (Cnudde & Boone, 2013). Within a predefined time interval, they were scanned to see two reaction products: the evolution of the production and magnitude of nitrogen gas and microbiologically induced calcium carbonate precipitation. This technique made it possible to create a 3D grain and pore network model of the samples immersed with the bacteria. Not only did it show the different locations of nitrogen gas and newly deposited calcium carbonate, but also how this evolved over time and how this affected the grains and pore network. Due to this changing pore network, changes of the water flow within the samples are generated which influence their weathering behaviour. Furthermore, it also resulted in a better understanding about how limestone, with a completely different pore network, influences the activity of the bacteria and vice versa.

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X-ray microtomography imaging of biofilms in porous media

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Bacteria often develop in sessile colonies at the interface between two phases - and mostly on solid surfaces - where the micro-organisms are embedded in a complex self-secreted polymer matrix. Such colonies, called biofilms, provide the nested bacteria with a better resistance to various environmental stresses including predators and biocides. Biofilms are ubiquitous[1] in our lives and form on catheters and prostheses, in water pipes, soils and aquifers, especially in the hyporheic zone where they play an important role in biogeochemical fluxes. When developing in a porous medium, biofilms can induce significant changes to the medium's transport properties (porosity, permeability, dispersion) with implications in many engineering and medical applications (e.g. biofilters, soil remediation, MEOR[2], CO2 storage, biofilms orthopaedic infections[3]). Still, the vast majority of processes controlling the growth of biofilms in porous media are poorly understood; this includes the impact of environmental constraints on spatial distribution of micro-organisms, the relationship between the various scales involved and the behaviour of biofilms in severely disrupted environments. This lack of understanding about the fundamentals of biofilm development in porous media is mostly due to the limits of currently used imaging methods.

Confocal laser scanning and multi-photon microscopy, which are widely used techniques for biofilms, allow for imaging with micron accuracy on a flat surface. However, application of these methods to a porous (and generally opaque) structure is extremely limited. Although magnetic resonance imaging techniques are rapidly advancing, this method does not currently provide sufficient isotropic spatial resolution. Approaches based on X-ray microtomography are also being explored as this technique theoretically enables the imaging of large volumes of porous media with submicron resolution. However, X-ray absorption coefficients for the biofilm and the surrounding aqueous phase are very similar and therefore contrast agents must be used to differentiate between phases.

Contrast agents such as silver-coated microspheres[4], 1-chloronaphtalene[5] and barium sulfate (BaSO4)[6] have been tested, but currently each of these has drawbacks restricting their application. In an extension to Davit et al. 2011[6] in which BaSO4 was used to provide a sharp contrast between the different phases of the medium, we will present a method which employs low-gelling temperature agarose gel to overcome sedimentation problems. This approach is validated against two-photon microscopy of biofilm growth in capillaries by comparing 3D surfaces and volumes extracted from both imaging modalities. The contrast agent is shown to be space filling and enabled a clear 3D visualisation of the biofilm contour with a smaller uncertainty on quantitative metrics than two-photon microscopy.

We will also demonstrate how this approach can quantify both biofilm distribution in pore space and biofilm morphology for different growth conditions in 3D-printed porous media models. The use of 3D printing allows porous structures with known properties (porosity, permeability and pore size) to be replicated. This enables experimental study of biofilm growth with only one varying parameter (e.g. flow rate, nutrient concentration or oxygen concentration), revealing its influence on the biofilm architecture inside the porous network.

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A Novel Approach for Characterizing Two-Phase Fluid Flow Experiments by Means of Continuous NMR Monitoring

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Nuclear magnetic resonance (NMR) is a well established laboratory / borehole method to characterize the storage and transport properties of rocks due to its direct sensitivity to the corresponding pore fluid content (water / oil) and pore sizes. Thereby, the correct estimation of these properties depends strongly on the calibration of the underlying pore model. Here, we combine a novel inversion approach that uses an angular pore model and different levels of saturation to directly determine the pore size distribution of the sample without the need of the aforementioned calibration. We present results of state-of-the-art two-phase flow experiments in a high-pressure NMR flow cell carried out on tight gas sandstones. The samples are installed at high confining pressures and are initially fully water saturated. Subsequently, the samples are drained with nitrogen gas by applying increasing differential pressures and the relative gas permeabilities are measured. The whole drainage process is monitored by NMR relaxation measurements to continuously determine the saturation of the sample. This allows for a direct estimation of saturation dependent relative permeability, a key parameter when estimating production rates of reservoir rocks.

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Computational modeling of nuclear magnetic resonance relaxation mechanism in hydrocarbon-bearing porous media using the seismic attributes

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Fractured carbonate reservoirs are identified as dual porosity porous media which possess a very complicated pore space structure [1]. Such a complexity poses significant challenges on studying and examining fluid flow patterns in these media. However, in recent years, nuclear magnetic resonance (NMR) has improved our understanding of the pore structure and fluid flow conditions in different types of porous media including fractured oil and gas reservoirs. NMR technology runs based on the fluids within the porous media [2]. In oil and gas engineering measurements, NMR acts on the basis of the longitudinal (T1) and transverse (T2) relaxation of the protons within the oil or gas molecules inside the pores. In this research NMR T1 and T2 relaxation mechanism are computationally modeled using the 3D post stack seismic response of the subject rock media as the input model parameters. Within the subsurface rocks, the seismic waves travel through the solid matrix and fluids inside the reservoir rocks. Therefore, the recorded seismic response will have a contribution of the fluids which relax when subjected to an external magnetic field and produce the magnetic resonance response. This is the key point that how two intrinsically different responses of the reservoir rock media, that is, the NMR and seismic responses, would be related. Therefore, extracting the relationship of the porous formation's seismic and magnetic resonance responses would help in predicting the relaxation phenomena that would happen in the unforeseen medium of the same type and conditions which specifically is the unforeseen section of the gas reservoir in this research. Additionally, by modeling the relaxation phenomena in the porous media, like the carbonate reservoir herein, we can predict the porosity and permeability of the media in presence of different fluids. In the current research the longitudinal and transverse relaxation phenomena are mathematically modeled in a fractured carbonate gas reservoir layer using statistical algorithms namely Bag ensembles and least square boosting ensembles. Meanwhile, this approach is introduced as a novel technique for obtaining NMR-derived permeability values in hydrocarbon-bearing geological formations. Nuclear magnetic resonance is a highly reliable tool in studying these media [3]; however, the required time and costs have always been the two major challenges for employing this technology. These challenges are solved by the proposed technique through manipulating the seismic data that is widely-accessible in the oil and gas fields. The proposed technique also provides the inexpensive estimation of T1/T2 ratio that helps to characterize the rock fluid system and also easily identify the signal of low-pressure gas when its T2 range overlaps with that of water [4]. The obtained results indicated that in the final models, the correlation of the measured and simulated relaxation values were more than 80% for both of the T1 and T2 values. This means that the proposed technique acted successfully in simulating the NMR relaxation phenomena and could be counted on for further up-scaling purposes.

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Exploring weathering process in natural building stones by portable NMR

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The application of NMR method to Cultural Heritage is relatively recent; several studies have demonstrated the potential of the method in describing the porous structure of materials employed in archeological and historical artifacts [1]. An important field of research in Cultural Heritage concerns building stones and the investigation of aspects related to modification of pore structure due to weathering and the application of conservative treatments, usually difficult to inspect in non invasive and non-destructive way. Effectively, NMR can be considered an efficient probe to study the aforementioned aspects in porous stones [2-4]. In this contribute, we present the results of an experimental study finalized to inspect the potential of portable unilateral NMR device in describing and quantifying the variation in pore size distribution of natural building stones due to weathering process induced by salt crystallization. In particular, a portable NMR sensor (NMR-Mouse®, RWTH Aachen University) [5] has been used to obtain in a fully non-invasive and non-destructive way, information about average porous radius, the pores interconnections and the distribution of pores of water-saturated unweathered and artificially weathered building stone samples. In detail, a coarse grained calcarenite from Sabucina (Caltanissetta, Sicily, Italy) widely used as building and replace stone in Sicilian ancient masonry has been selected for the measurements. In order to obtain petrophysical parameters such us the total open porosity, the surface-to volume ratio, the average porous radius, the tortuosity factor, the pore size distribution, both T2 relaxation time (CPMG) and diffusion measurements (Steady gradient stimulated echo, SGeneral Session TE) have been carried out at different depth within the stone sample. Furthermore, to exclude in our case the diffusion coupling between pores in Sabucina and to verify that T2 relaxation time distribution reflects the pore size distribution, a comparison with the mercury injection curves (MIP) have been performed. The obtained results have highlighted a shift of T2 more populated component from shorter to longer times with the advancement of weathering process, with trend perfectly in accordance with previous studies in which the effect of weathering mechanism in pore structure of building stones has been investigated by applying destructive methods [6].

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PFG-MRI of flow, diffusion and exchange in complex porous bio-systems

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Pulsed Field gradient (PFG) NMR and MRI methods have been successfully applied to study flow in (complex) porous media. Exchange between water in different ((sub)cellular) compartments and flow conducting structures is an important factor to be considered in quantifying flow in porous biosystems like e.g. tissues (tissue perfusion), (woody) plants and bio(film)-reactors. These porous biosystems are characterized by complex (dispersive) flow, and exchange between flowing and stagnant fluid pools, with surface relaxation effects, internal field gradients due to susceptibility differences and differences in relaxation times between exchanging flowing and stagnant water pools. Pulsed field gradient (PFG) MRI propagator methods can be used to measure spatially resolved complex flow, even in pixels that contain both flowing and stagnant fluid [1,2,3]. The discrimination of flowing and stagnant fluid and the determination of flow characteristics are, however, not straightforward in general, and certainly not if exchange between these pools is present [4]. Combined 2D correlation spectroscopy MRI methods like diffusion-T2, T1-T2 and flow-T2 [5] can be used to characterize the water dynamics in such porous biosystems. Doing so, it is possible to quantify exchange and the effect on flow parameters and diffusion. This will be illustrated in a number of porous biosystems: xylem and phloem transport in (woody) plants and transport in bio-reactors, containing flow and transport in biofilms fixed on beads or in granules (e.g. waste water bioreactors). In the xylem of (woody) plants isolated or clustered flow conducting vessels are surrounded by tracheids and parenchyma cells, containing stagnant water. Water in the different environments has different relaxation times. Exchange between these environments is important for the coupling between water in storage pools and the flow conducting vessels. These storage pools have a function in buffering water transport fluxes during daily fluctuations in water demand and during seasonal water deficits to prevent unfavorable stress effects. In the phloem, transport of photoassimilates is in the sieve tubes. This pathway couples source and sinks. Although essential for growth and optimal functioning it is one of the least understood plant processes. By MRI flowmetry we have demonstrated that phloem transport is regulated on velocity, by (de-)activation additional sieve tube transport if necessary to de- or increase the flow [6]. In bioreactors combined flow-T2 MRI can resolve the flow of the medium and transport in the biofilm at a pixel level. MRI is at present the only method that allows studying these parameters.

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A Model for the Sorption Kinetics of Salt/Zeolite Composites

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Impregnation with salt is a promising way to raise the energy storage density of zeolite-based thermochemical heat storage materials significantly (e. g., increases of 27 % [1] and 48 % [2] have been reported). However, in doing so, the fast adsorption kinetics of the zeolite is accompanied by the slow absorption kinetics of the salt, which means that the kinetics become a limiting factor in the heat storage process. The sorption kinetics of a composite sorbent material are an important parameter for the layout of an application-scale reactor, which should provide an overall heat power in- and output comparable to a reactor operated with pure zeolite.If the slower sorption kinetics is not accounted for, the temperature lift in the reactor will decrease over time, whereby the necessary output temperature will not be reached anymore, even though the heat storage material is not fully discharged yet. We present a phenomenological model of the sorption kinetics of a salt-impregnated zeolite, which complements an already existing model of the sorption equilibria of said composites [3]. The modelling focuses on zeolite-X impregnated with sodium chloride, calcium chloride, magnesium chloride or magnesium sulphate. It describes in particular the dependence of the kinetics on the salt content. Our modelled kinetics can be used to find suitable sorbent material parameters, reactor dimensions or operating conditions in numerical simulations of thermochemical heat storage devices (for a review of such modelling cf. e. g. [4]).

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Modelling and simulation of the heat and mass transfer in an adsorber of a closed low-pressure adsorption system for thermal energy storage

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The realization of a sustainable as well as ecological and economical energy supply requires the development of efficient energy storages. One promising storage concept is given by thermal energy storages based on adsorption [1]. Against this background, this work deals with the modelling and simulation of the heat and mass transfer in an adsorber (zeolite 13X / water) of a closed low-pressure adsorption system for thermal energy storage.

Especially, the adsorption process (discharging mode) is of particular interest. The challenges regarding modelling and simulation follow from the special characteristics of low-pressure adsorption systems. For such systems, spatial and temporal variable flow regimes with different dominating physical effects exist simultaneously ($0.01 < Kn < 10$). Furthermore, the examined system poses a multi-scale problem. The three most relevant scales can be defined as the macro scale (whole storage), the meso scale (adsorbent particle cluster) and the micro scale (single particle).

In this work a simplified model is formulated on the meso scale to gain insights on the macro scale behaviour. Three different mass transport approaches (no-slip (Darcy), slip (Klinkenberg), Sharipov [2]) are implemented and examined. Further, the heat transport and the water uptake behaviour are discussed. The present communication will discuss our assessment of the relevance of the different flow domains and of the different mass transport approaches. Furthermore, this works contributes to the ongoing discussion in the field whether such processes are limited by the heat or mass transfer [3]. For this purpose, simulations are performed over a wide range of geometry and process parameters and the results are summarized in comprehensive diagrams.

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Numerical Model of a CaO/Ca(OH)2-heat storage reactor

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Thermochemical heat storage has a large potential due to its high storage density [1]. In the range of high to medium temperature heat storage the system Calciumoxide – Calciumhydroxide is of special interest, as it reacts at handable temperatures (300-500 °C), is environmentally friendly and financially attractive [2]. The following chemical reaction is considered:

$CaO(s) + H2O(g) \leftrightarrow Ca(OH)2\ (s) + \Delta HR$

In order to develop a technical application, the processes of the chemical reaction have to be investigated: The granular material (CaO/Ca(OH)2) undergoes a volume change so that its porosity and permeability and thus the flow processes of the heat transfer fluid are changed [1]. Furthermore, the reaction kinetics and the cycling stability have to be examined further. To understand the processes and estimate their relevance on the different scales, a 2D numerical model is built in the open-source simulator DuMuX [3] on the REV scale. The constitutive relations of the complex system are depicted in a multiphase system. Changes in the structural properties such as porosity and permeability are considered as well as thermal non-equilibrium.

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A new borehole testing methods using granular polyacrylamide gel as temporary sealing material

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The range of options for investigation of hydraulic behavior of aquifers from boreholes has been limited to rigid, cumbersome packers, and inflatable sleeves. Here we propose a new temporary borehole sealing technique using soft grains of polyacrylamide gel as a sealing material and discuss its possible applications. If no compressive stress is applied, the gel packing (permeability similar to open gravel) suppresses free convection, allowing for local temperature and chemical sampling through free-flowing gel. Minimizing the effect of free convection within the well column would be beneficial for active thermal tests where free convection often dominate flow and create thermal disequilibrium between the water in the borehole and the surrounding media. Preliminary laboratory study and the literature suggests that as the polyacrylamide pack is subject to modest compressive stress to the gel media (of order 0.1 ATM), the permeability transitions from of the order of 10^7 millidarcys to 0.01 millidarcys, illustrating the remarkable ability to transition from highly permeable to nearly impermeable grouting. Though yet to be confirmed in the field, by locally injecting water at pressure greater than the compressive stress, local voids can be formed which can act as local pump test sources, with all other locations in the borehole hydraulically isolated where local response pressure from the formation can be measured. This arrangement could be valuable for tomographic study of aquifers wherein hundreds of injection zones could be tested by simply pulling an injection pipe vertically through the packed borehole. The gel grains can be of the scale of cm, so do not pass through well-screens or enter fractures of mm scale. When compressive stress is relieved, the PAM media is easily pumped out of a well with standard equipment.

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Experimental investigation and numerical simulation of non-Newtonian flow of bentonite suspension through porous media based on a pore space description gained from µCT analysis

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In this study, numerical simulations are verified with laboratory tests to investigate the flow behavior of bentonite suspensions through the pore space of coarse media. The coarse media are provided by packed glass beads with diameters of 2mm and 600-850µm. The geometrical description of the pore space has been acquired by scanning different samples of the glass beads using µCT. By applying AVIZO software for image processing, a 3D network of the pore space is generated. Based on the 3D model the connected and unconnected pores are depicted. The definite size and shape of the "real" geometry is transferred in a generated mesh of the pore space (see Figure 1). In a second step, the flow field is solved using finite volume method. It includes the generation of the mesh of the fluid region using ICEM and setting the boundary conditions. These exhibit the inlet and the outlet flux and the stationary walls. The open source software openFOAM is applied to solve transient, incompressible, laminar flow for non-Newtonian fluids. Simulations of the flow in the definite pore space are conducted in several steps by increasing the complexity of the applied fluid model: at first, the flow of Newtonian fluid without yield stress is modelled followed by applying viscosity parameter to the characteristics of the fluid. Afterwards, the modelling of non-Newtonian fluid is performed by adding the yield point parameter and the non-linear relation between shear rate and yield stress. For modelling the bentonite suspension, in a first step the Bingham approach is used. In a next step, the more advanced Herschel-Bulkley model is applied. Here, numerical methods, such as finite volume in conjunction with computational implementation are utilized. As a result of this simulation the pressure field in the porous medium is obtained. This is compared to the results gained from the laboratory experiments. The experiments are performed using the packed glass beads of diameters 2mm and 600-850µm in a cylinder. The fluids are injected through these beads in certain velocities meanwhile the pressure drop is measured at several positions within the flow area. Verification of simulation is conducted by comparing the values of velocity as a function of pressure gradient with the experimental values.

Figure 1: Separation of the elements of porous media: tetrahedral mesh of the pore space (left) and of the glass beads (right) using AVIZO

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Flow behaviour of partially hydrolysed polyacrylamide polymers in granular soils

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Partially hydrolysed polyacrylamide (PHPA) based polymers are used in a variety of civil engineering applications including as excavation support fluids in construction work such as piling and borehole drilling. For these applications, the role of the fluid is to keep the excavation open during digging. PHPA based polymers offer promising solutions to challenging problems such as stabilising coarse grained soils. They also require a smaller site plant set-up than conventional bentonite clay based support fluids and can show reduced environmental impacts. However, there are problems, for example, excessive loss of polymer from the excavation by permeation of the fluid into the adjacent ground. This is not only detrimental to excavation stability but also wastes polymer. To tailor polymers to meet the demands of specific engineering projects it is necessary to develop a fuller understanding of their flow and sorption behaviours. The research presented sets out the results of some tests to develop the understanding of the underpinning science as related to the rheological and sorption behaviour of polymers fluids in coarse grained soils. The results of a series of laboratory studies of the flow of PHPA polymer fluids in sands over a range of grain sizes and pressure heads will be presented. The data were obtained using a constant head permeability set-up modified to obtain data over a range of depths into the sand bed. In parallel, theoretical aspects of polymer fluid flow in porous media have been revisited and applied to obtain a better insight into the underpinning microscopic and macroscopic phenomena involved. Measurements made under steady-state flow conditions showed that depending on the concentration of active polymer in solution, the soil hydraulic conductivity (i.e. Darcy permeability rather than intrinsic permeability) to polymer fluid is much lower than that for water. The validity of a capillary bundle model to explain the observed behaviour was tested against the experimental data. The results indicate that such a model is inadequate to address the rheological behaviour of the PHPA polymer solutions in soil pores. To fit the porous media data to a capillary bundle model would require that the power law flow index for the fluids should be varied with capillary diameter as estimated from the sand grain size. Furthermore, the experimental results show a zone of reduced hydraulic conductivity in the first tens of mm into the sand bed implying there may be polymer sorption occurring in this zone. Uncertainties regarding the theoretical description of polymer fluid flow in coarse grained soils using capillary model will be further discussed. The microscopic interactions of polymers and solid particles showing a profound effect on the macroscopic flow process in sand also will be presented.

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GRAVITY CURRENTS OF HERSCHEL-BULKLEY FLUIDS IN A POROUS MEDIUM: ANALYTICAL MODELS AND EXPERIMENTS

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The aim of this paper is to study gravity currents of rheologically complex fluids in porous media. Two-dimensional motion of a shear-thinning/thickening fluid with a yield stress (described by the Herschel-Bulkley model) in a narrow fracture slumping under gravity is investigated analytically, numerically and experimentally, extending the work by King & Woods [1], Longo et al. [2] and Ciriello et al. [3]. A modified version of Darcy's law is assumed to describe the motion of the gravity current, whose volume is taken to vary as a monomial function of time. A closed-form self-similar solution is derived for a fluid volume that scales as time squared. This solution reveals that for injection rates scaling at a rate slower than time, the current will eventually evolve to consist entirely of plug flow (ignoring any three-dimensional disturbances caused by fluid injection). Therefore gravity currents formed either by a finite release of fluid, or by a constant fluid injection rate must eventually drop below the yield stress and consist completely of plugged fluid. For a generic increase of the volume of the gravity current with time, the propagation is studied numerically with an ad-hoc code. The availability of a closed-form self-similar solution allows an immediate verification of the model and a validation of the experimental set-up. For a discharge rate linearly increasing in time, the profile of the current is linear and the velocity of the front of the current is constant. Two series of experiments have been successfully completed: i) direct simulation of the current propagation in an artificial porous medium composed of a homogeneous layer of glass beads, and ii) indirect simulation in an Hele-Shaw analogue model. The fluid used in the experiments is a neutralized mixture of deionized water and Carbopol 980, added with ink for an easy visualization. The rheometric parameters have been measured with a shear stress controlled rheometer with parallel plates. A specific effort has been devoted to measuring the yield stress, which is a well-known difficult task. A series of dynamic tests, creeping and relaxing tests, and direct measurement tests with a tilting plane have been performed for achieving a consistent validation of the yield stress measurements. A last critical aspect is the wall slip which affects many polymer fluids flows, especially if a yield stress is present. While slip does not affect the flow in the direct model, it modifies the measurements in the rheometer and the Hele-Shaw cell tests. To quantify the slip effect, the plates in the rheometer have been roughened with sand paper, and the internal walls of the Hele-Shaw cell have been roughened with transparent anti-slippery ribbons for stairs. The overall conclusion is that the theoretical model is well interpreting the flow of the current in the intermediate asymptotic regime, far from the injection section (where three dimensional effects are quite evident) and in the limit of the thin current approximation. Moreover, the rheological behavior of the HB fluid in the porous medium is well described by the present model.

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Modeling and Simulation of polyurethane foam injection moulding to produce fiber reinforced sandwich structures

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Rigid polyurethane foam (PUR) reinforced with warp-knitted spacer fabrics offers a high potential for application as lightweight sandwich construction due to the textile structure of the spacer fabric. Two textile surfaces, held by monofilaments at a defined distance, are filled by the PUR foam by a reaction injection molding process. The simulation of the propagation characteristics of PUR is an industrial application of complex Non-Newtonian flow in permeable media and is of vital importance for prediction of the local foam density of the sandwich construction and for finding appropriate process parameters. The modeling of the flow behavior of PUR foam through textile structures additionally has to consider the local flow resistance as well as the correct tracking of the foam front. Both, the local resistance as well as the correct front propagation through the porous structure is studied by microstructure analysis and simulation to obtain effective macroscopic model parameters. Then, a coupled system of partial differential equations consisting of Navier-Stokes-Brinkman equation and a Volume of Fluid formulation for the free surface is solved in the mould. Time and temperature depending viscosity as input parameters for the model are determined by rheological experiments. Mold filling experiments as well as combined foam expansion and rheometer experiments validate the developed models. The results help engineers in the mold design and adjustment of process parameters as well as understanding of porous media flow of expanding polyurethane foams mixtures.

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Non-linearities in yield stress fluid flows through porous media

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The flow of yield stress fluids (foams, emulsions, concentrated suspensions) through porous media is of interest for injection of muds, slurries or cement grouts to reinforce soils or structures, or in oil recovery processes. Since such materials exhibit a strongly non-linear constitutive equation, i.e. they behave as liquids above a critical stress and as solids otherwise, specific, possibly non-linear, flow characteristics in through porous media may be expected. This starts with the "Darcy's law" (namely pressure vs mean velocity equation) for such fluids: a non-linear relationship is expected, since no flow can occur below a critical pressure; its experimental determination is a challenge in particular because usual techniques for determining the pressure may fail when applied to complex flows possibly exhibiting solid and liquid regions. However careful experiments show that the Darcy'law expresses as a critical pressure value to overcome to get a flow and a pressure vs velocity equation in the liquid regime with a form similar to that of the constitutive equation of the fluid. Systematic tests varying the fluid and porous medium parameters confirm the expected scaling of the parameters of this Darcy's law [1]. The question of the physical origin of such a law and of its coefficients nevertheless remains open. It was suggested that such flows exhibit two original trends: as the pressure drop increases a wider region of fluid starts to flow, an effect occurring at a local scale; at a macroscopic scale the flow starts only along a specific path throughout the porous medium and as the pressure drop is increased more flowing paths progressively form within the porous medium [2-3]. Such trends are in agreement with the flow characteristics through a single model pore (of larger diameter than the entrance and exit conduit) observed by MRI: the fluid flows through the pre-existing fluid almost without disturbing it, which essentially remains at rest except in a thin (shear-band) layer [4]. However, with a simple porous medium (granular packing), from measurements using a NMR technique (pulsed-gradient spin echo (PGeneral Session E)) not affected by spatial resolution problems, it was shown [5] that the probability density function of the velocity is similar to that for a Newtonian fluid, which suggests that this is the same for the local velocity field. This result was confirmed by numerical simulation of 2D flow through disk packing [6]. This suggests that these results obtained for strongly non-linear fluid can be extrapolated to any non-linear fluid. From the similarities observed for the velocity distribution for different pore sizes and flow rate we deduce a generalized form of the Darcy's law for such materials and provides an insight in the physical origin of the coefficients involved in this expression, which are shown to be moments of the second invariant of the strain rate tensor.

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On the determination of a generalized Darcy equation for yield stress fluid in porous media

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Non-Newtonian fluids have practical applications in very different domains. Indeed, polymer mixture, paints, slurries, colloidal suspensions, emulsions, foams or heavy oil present complex rheologies. Among the large number of different non-Newtonian fluids an important class of behavior is represented by the yield-stress fluids, viz. fluids that require a minimum of stress to flow. Yield stress fluids are usually modeled as a Bingham fluid or by the Herschel-Bulkley equation.

However, simulating the flow of a Bingham fluid in porous media still remains a challenging task as the yield stress may significantly alter the numerical stability and precision. In the present work, we use a Lattice-Boltzmann TRT scheme to determine this type of flow in a synthetic porous medium or fracture. Different pressure drops dP were applied in order to drive the fluid. On the figure different velocity fields are represented as a function of dP. Close to the threshold, dP_c, the fluid is flowing in only few paths. For a pressure difference higher than several orders of magnitude, one observe that all the fluid in the medium is now flowing. We then determined a generalized Darcy equation by evaluating the flow in the porous structure. Three different scaling regimes can be distinguished as function of the distance to the critical pressure dP-dPc. Regime I corresponds to the situation where the fluid is flowing in only one channel. Here, the relation between flow rate and pressure drop is given by the non-Newtonian Poiseuille law. During Regime II, an increase in pressure triggers the opening of new paths. The relation between flow rate and the difference in pressure to the critical yield pressure becomes quadratic. Finally, Regime III corresponds to the situation where all the fluid is sheared. In which case one have a linear relationship between the flow rate and the applied pressure.

In this presentation, we will investigate the crucial importance of the heterogeneities on these flowing regimes. In particular, we will demonstrate that the statistical distribution of the unyielded regions follows a power-law. The exponents are able to account for the transition between the regimes but also on the different pressure-flow rate relationships. Finally, we will propose a simple model, based on pore network and avalanche dynamic, which is able to predict the correct statistics and exponents.

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POROUS GRAVITY CURRENTS OF NON-NEWTONIAN POWER-LAW FLUIDS: A REVIEW OF THEORETICAL AND EXPERIMENTAL RESULTS

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The study of gravity currents within porous media is motivated by the need to model environmental and industrial processes in which an intruding fluid propagates inside a porous medium saturated with another fluid [1]. While the body of knowledge accumulated on gravity driven flows in porous media concerns mainly Newtonian fluids [2,3], real flows often involve fluids with complex rheology. Relevant applications include, but are not limited to, environmental contamination and in situ remediation. The aim of this paper is to present a review of the theoretical and experimental results obtained by our group concerning the modeling of porous gravity currents of power-law fluids of index n. The propagation of thin currents over a horizontal, rigid and impermeable bed inside a porous domain saturated with an ambient fluid is considered under the sharp interface schematization. The volume of the advancing current is taken to vary as a power function of time with exponent α. First, closed form results were obtained for gravity currents propagating in plane or cylindrical geometry, deriving scalings for current length and thickness as functions of n and α [4-6]. Based on these benchmarks, the analytical models were refined introducing additional factors: medium heterogeneity and topographic control. On one hand, the inherent heterogeneity of natural media was modeled [7-9] considering continuous variations of spatial properties described by simple power-law relationships, in the vertical or horizontal direction. Vertical variations mimick stratifications of natural media, while horizontal variations represent e.g. permeability alterations occurring nearby an injection well and induced by the drilling process. To analyze this configuration, novel results concerning spreading in radial geometry were obtained when the medium permeability varies along the propagation direction. On the other hand, topographic control was modeled considering flows in porous channels of different shapes [10]. Both heterogeneity and topographic control proved relevant for the spreading of gravity currents as they influence the extent and shape of porous domain invaded by the contaminant, or reached by the remediation agent. Our theoretical results were validated against multiple sets of experiments, conducted with different combinations of spreading scenarios and types of heterogeneity or channelization. Two basic experimental setups were employed, adopting either reconstructed porous media made of glass beads, or Hele-Shaw analogues. To this end, existing Hele-Shaw analogies for porous flow of power-law fluids were extended to heterogeneous media. All scalings derived for the current front and thickness were confirmed by our experiments, with an agreement between theory and experiments improving with time, due to the limitations of the thin current approximation and boundary effcts near the injection zone. A comparison between the key exponents governing the propagation of the gravity current allows to determine the relative influence of rheology, heterogeneity, domain shape and geometry. The limitations on model parameters imposed by model assumptions are discussed in depth, considering currents with increasing/decreasing velocity, thickness, and aspect ratio, and their sensitivity to model parameters. Multiple critical values of the injection exponent α discriminating between opposite tendencies are thus determined.

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RAYLEIGH-BÉNARD INSTABILITY OF THE POWER-LAW FLUID FLOW IN A POROUS MEDIUM: NUMERICAL AND EXPERIMENTAL ANALYSIS

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The thermal instability of fluid saturated porous media is a topic extensively investigated in the last decades. The scientific community has focused its efforts especially on the study of the stability of Newtonian fluids [1]. The investigation of the stability of non-Newtonian fluids is a topic poorly explored. Only a few papers extended the results reported by Horton and Rogers [2], Lapwood [3], and Prats [4] to non-Newtonian fluids. The aim of this paper is to further develop the work done by Barletta and Nield [5] with reference to a fluid characterised by a temperature-dependent consistency index. A two dimensional fluid saturated horizontal porous layer is thus investigated with respect to the onset of thermal instability. The porous layer is subject to a horizontal throughflow and it is heated from below as in the classical Prats problem. A power-law fluid is considered. An extended Darcy's law and Oberbeck-Boussinesq approximation are assumed while the solid phase and the fluid phase are in local thermal equilibrium. A temperature-dependent viscosity model is employed. The porous layer is impermeable. Two different temperatures are imposed, with heating from below. The problem here described is investigated both numerically and experimentally. From the theoretical viewpoint, the stationary basic throughflow is perturbed by plane wave disturbances. A linear stability analysis is thus carried out using the normal mode method. The eigenvalue problem obtained is solved numerically by means of the Runge-Kutta method coupled with the shooting method. The neutral stability curves are obtained along with the critical values of the stability parameters that identify the threshold for the onset of thermal instability. The experimental configuration employed for the analysis of this problem consists of a Hele-Shaw cell. The cell is composed by an aluminium frame with a central window obtained by using two polycarbonate plates that ensure the optical access to the cell for velocity measurements. These measurements are performed with a Particle Image Velocimetry (PIV). The isothermal boundary conditions are obtained by circulating water for the hot lower boundary, and by circulating coolant for the cold upper boundary. Two free surface wells are connected to the cell, allowing injection and extraction of fluid in order to generate a constant horizontal flow. A syringe pump is used to inject the requested discharge inside the cell. The pump discharge is modulated by a Proportional Integral Derivative (PID) control system. In order to obtain a purely vertical temperature gradient, the cell is thermally insulated in all its components with foam rubber and thermal insulating tape. The experimental investigation poses several challenges, such as the choice of tracers for PIV measurements, the discrimination between horizontal velocity components induced by convection and the imposed throughflow, the presence of hysteretic effects in cell appearance and disappearance, and the correct reproduction of shear-thickening behaviour.

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Scale Effects in the Flow of a Shear-Thinning Fluid in Rough Fractures

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The understanding of flow processes involving non-Newtonian fluids in the subsurface is of interest for many engineering applications, from in-situ remediation to enhanced oil recovery. The fluids of interest in such applications (f.e., polymers in remediation) often present shear-thinning properties, i.e., their viscosity decreases as a function of the local shear rate. We investigate how fracture wall roughness impacts the flow of a shear-thinning fluid. Numerical simulations of flow in 3D fracture geometries are carried out by solving a modified Navier-Stokes equation incorporating the Carreau viscous-shear model. The synthetic fractures consist of two rough surfaces which are isotropic self-affine geometries and correlated with each other above a scale which we denote correlation length (see Méheust et al. PAGEOPH 2003). Perfect plastic closing is assumed when the surfaces touch each other. The objective is to test how varying the correlation length impacts the flow behavior, for different degrees of closure, and how this behavior diverges for shear-thinning fluids from what is known for Newtonian fluids. The results from the 3D simulations are also compared to 2D simulations based on the lubrication theory, which we have developed as an extension of the Reynolds equation for Newtonian fluids. We also discuss the implications of our results for the general understanding of the flows of shear-thinning fluids in fractured media and of solute transport by such flows.

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Shear Thinning Flow Behavior of Aqueous Colloidal Silica Suspensions and Its Application in Amendment Delivery for Subsurface Remediation

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Owning to the shear thinning flow characteristics of the fresh colloidal silica (fumed silica) suspensions and their sequential gelation rheological behavior, these suspensions are being tested for their feasibility to be used as carriers for remedial amendment delivery in subsurface remediation. The knowledge on the flow behavior and the influence of environmental conditions on the shear thinning of the suspensions is lack in the literature while it is essential for the manipulations of these suspensions. In this study, the influence of silica particle concentration, water source, ionic strength, pH, aging, amendment type and concentration, and subsurface sediment on the rheological behavior of the suspensions was investigated. All tested suspension formulations exhibited shear thinning before gelation. Higher silica particle concentration and salinity (Na+ and K+) increased suspensions' viscosity and the degree of shear thinning. The viscosity of suspensions increased with aging. Addition of KMnO4 amendment to aqueous silica suspensions increased viscosity, while addition of alcohol amendment decreased suspensions' viscosity. Mixing of colloidal silica into vegetable oil remarkably increased the viscosity of oil and rendered the shear thinning behavior of oil. The presence of amendment did not reduce shear thinning. The gelation rate of silica suspensions was increased with silica concentration and with the addition of sediments.

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Shear thinning fluids to optimize the injection of engineered microparticles for groundwater remediation

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Nanoscale and microscale zerovalent iron particles (NZVI and MZVI) are promising materials for the remediation of contaminated aquifers [1]. These particles are dispersed in water-based slurries and injected in the subsoil to generate a reactive zone. However, the successful injection of MZVI and NZVI may be significantly hindered by the reduced colloidal stability, and therefore mobility in the porous medium, due to the fast sedimentation (MZVI) and aggregation (NZVI) of the particles when dispersed in water [2-4]. To overcome this issue the use of stabilizing agents wax proposed: shear thinning solutions of green biopolymers have been recently studied as kinetic stabilizers and viscous carrier fluids for the delivery of MZVI and NZVI [3]. Shear thinning fluids exhibit high viscosity in static conditions, improving the colloidal stability, and lower viscosity at high flow rates enabling the injection at limited pressures [5]. In this work the use of guar gum is presented. Polymeric solutions (1.5 to 7 g/l) were prepared following different procedures, and their efficacy in stabilizing highly concentrated dispersions of MZVI (20 g/l, average size 1.2 um) was evaluated. Ideally, the optimal guar gum suspension should (i) keep the MZVI suspended for a time sufficient for its injection; (ii) be easily degradable, to avoid possible negative effects on MZVI reactivity; (iii) do not clog the porous medium due to residual undissolved guar gum. With these targets in mind, a detailed rheological characterization of the guar gum, both in the bulk and when injected in a porous medium, was carried out. A modified Cross model, linking guar gum concentration and bulk shear viscosity, was derived based on bulk rheological measurements. Column filtration tests were then performed, and a modified Darcy law was derived to predict pressure gradients arising during guar gum injection. The kinetics of guar gum degradation was studied to investigate the correct enzymes dosage required to achieve a complete breakdown of the suspensions, and a modified Stokes law for the prediction of the sedimentation rate of the MZVI was proposed and validated. All derived empirical relationships (namely, rheological model, modified Stokes law and Darcy law) were finally included in MNMs (www.polito.it/groundwater/software/MNMs.php), a software for particle transport simulation in 1D (column) and radial domain. MNMs can be used as a tool for a preliminary design of the field injection of MZVI/NZVI - guar gum mixtures, providing an estimate of particle transport and pressure build up associated to the injection at the pilot scale. Funded by: EU FP7 Aquarehab Grant Agreement No. 226565

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Chemical Weathering, Soil Formation, and Calcic Horizon Depths

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Scaling of non-Gaussian transport in percolation theory can be combined with deep infiltration rates (Precipitation, P, less Evapotranspiration, ET + run-on – run-off) and knowledge of particle size data to predict the typical solute transport distance as a function of time. This distance is found to equal soil depths for times from years to 100 million years. The derivative of the solute particle distance with respect to time gives the soil production rate, which is verified over time scales of months to 50 million years, and over precipitation rates from 0.002m/yr to 10m/yr. This derivative also gives the chemical weathering rate over a similar time period and is in agreement with the major metastudies of field data (White and Brantley, 2003; Maher, 2010). Other quantities predicted by this simple formulation include soil N and C sequestration rates as a function of soil age. In arid regions, where soil formation is minimal, but calcic and gypsic horizons are frequently found, the depths of these horizons is found to scale with P - ET exactly as predicted and without use of adjustable parameters. The research has recently been published in Water Resources Research. Consequences include the known greater soil depths in convergent, compared with divergent, terrain, a result echoed in the growth of trees. The same scaling relationship then also predicts infiltration more accurately than the Philip theory (separate presentation, invited featured publication in Water). Related predictions that link 12 orders of magnitude of time scales are verified in vegetation growth. Verified predictions in the geosciences connecting different processes over 15 orders of magnitude, and that do not use adjustable parameters, are rare, to say the least. Overpredicting the scaling exponent 0.53) by as little as 20% would cause an error of a factor 25, leading (for infiltration rates of 3m/yr and particle sizes of 10 microns) to predicted paleosol depths of 1400m at 50Myr instead of the observed 50m depths characteristic 1of bauxites and laterites. When predictions couple such widely different processes as soil formation and vegetation growth to the same fundamental pore-scale flow rates, this organizational capability is unprecedented.

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Intermittent burst dynamics during slow drainage flows

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The intermittent burst dynamics during the slow drainage of an artificial quasi-2D porous medium is studied experimentally. We have verified a theoretically predicted scaling for the burst size distribution (see figure) which was previously accessible only via numerical simulations. We show that this system satisfies a set of conditions known to be true for critical systems, such as intermittent activity with bursts extending over several time and length scales, self-similar macroscopic fractal structure and a scaling behavior for the power spectrum associated with pressure fluctuations during the flow. The observation of a 1/f scaling region in the power spectra is new for porous media flows and, for specific boundary conditions, we notice the occurrence of a transition from 1/f to 1/f^2 scaling. An analytically integrable mathematical framework was employed to explain this behavior.

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Measurement of the dynamical scaling for the pair correlation function during slow drainage of 2D porous media.

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An experiment were we have full access to the spatiotemporal evolution of the invasion front under drainage in a porous media is discussed. We have found experimental validation to the unusual dynamic scaling for the pair correlation function N (r, t), during slow drainage of a 2D porous medium, first observed by Furuberg et al. [1] nearly 30 years ago. We give a new theoretical argument for the scaling exponent of the short distances or long times and discuss the general scaling behaviour of N(r,t).

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Scaling Transpiration and Infiltration

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The dependence of vascular plant growth on water and nutrient sources in the soil places edaphic constraints on their growth rates. This growth is described in terms of a limiting diameter, x0, either xylem or pore, the pore-scale flow rate, v0, and an exponent, 1/Dopt = 1/1.21 = 0.82, from percolation theory that describes root radial extent, x, in terms of the actual root length, L = v0t, i.e., x = x0 (L/x0)^0.82 = x0 (t/t0)^0.82. Dopt is the 2D optimal paths exponent, since the root search is confined primarily to the topsoil. The equation was verified in dozens of tree studies (VZJ) with geometric mean x0 = 10µm and pore scale flow rates ranging from 20µm/s two orders of magnitude downward. At larger time scales I show (Fig. 1) that the same scaling relationship can be represented in terms of minimum and maximum values of transpiration across the spectrum from the Namibian desert (xg = 20mm per growing season, tg) to tropical savannahs and rainforests (xg = 1650mm) x = xg (t/tg) 0.82. The results explain simultaneously growth and growth rates of trees, roots, and clones, from 5 minutes to 100,000 years, as well as a number of recognized ecological puzzles, such as why trees grow more rapidly when young, in convergent topography, moister climates, and on wettable soils, rather than water-repellent soils or rocks. Given the success of a similar scaling relationship in terms of the infiltration rate (ranging from 20µm/s three orders of magnitude downward), soil particle diameter, 30µm, and 3D percolation backbone exponent, Db = 1.87, in predicting soil depths and soil formation rates, chemical weathering rates, and calcic and gypsic horizon depths out to 10^15s and over the entire range of Earth's climates (WRR), the corresponding scaling relationship for infiltration, I = (x0/t0) t + x0 (t/t0)^1/1.87, was tested (Water, invited, featured) on results of unsteady flow experiments by Sharma, and found to perform significantly better than Philip infiltration results, I = A t + S t^1/2 (Figs. 2 and 3). Here x0/t0 is again a pore-scale flow rate, effectively the saturated hydraulic conductivity. Fig. 1. BAAD database is compared with predicted upper and lower limits on growth rates using pore-scale flow rates discussed. Minimum and maximum scaling relationships could be equally expressed in terms of growing season limiting transpiration values, 20mm at the dry end, and 1650mm at the wet end, plotted on the graph at a six-month growing season. Fig. 2. Scaled infiltration vs. scaled time (Sharma et al. (1980). Blue and red curves are minimum and maximum expected from above theory. Philip's infiltration theory allows no scatter, and would, to within the resolution of the graph, coincide with the blue curve. Fig. 3. Percolation scaling (red) compared with data compiled by Sharma et al. (1980) for relationship between S and A. The observed data, exponent 0.727 (black line), is in agreement with percolation prediction, exponent 0.76 (in red), in contrast with Philip's infiltration theory, exponent 0.5 (in blue).

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Micro and Miniature Technologies for Advanced Passive Energy Systems (fuel cells and heat pipes)

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The 21st century will see the development of a wide range of active miniaturized energy devices with application in energy management and power sources, electronic cooling, energy storage and bioengineering. Although these active devices are effective, they are often cumbersome and inefficient considering the auxiliary supporting devices such as pumps, fans, and other moving parts they require for operation. A more efficient and novel approach involves the use of passive small energy and thermal devices with no moving parts. Two research thrusts are passive fuel cells and heat pipes which are discussed.

A Miniature passive direct methanol fuel cell (DMFC) that includes a fuel cell stack and ancillary systems with no moving parts will be presented. This system uses passive approaches for fuel storage and delivery, air breathing, water management, CO2 release, and thermal management. The performance characteristics of the passive miniature DMFC system will be presented.

Increasing component densities of the integrated circuit (IC) and packaging level, as well as energy conservation requirements have led to serious challenges in thermal management. Innovative heat pipes and thermosyphons are some of the most promising passive thermal devices because of their high efficiency, reliability and cost -effectiveness. Challenges and opportunities of these devices will be discussed.

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The poroelastic behavior of the human brain

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Our brain is one of the most fascinating—but undoubtedly also most complex—structures within our body. During trauma, stroke, or infection, an abnormal accumulation of fluid causes the brain to swell [5]. Within the limited space of the skull, brain swelling increases the intracranial pressure and reduces the supply of blood and oxygen. This can have devastating consequences.

Several theories and models have been proposed to explain brain swelling; yet, it remains controversial whether the brain should be viewed as a viscous fluid, an gel-like solid, or a multiphase material [2]. Here we review existing concepts and classify their usefulness in various clinical conditions. We provide experimental evidence that human brain tissue possesses multiple intrinsic time scales [1], which suggests that it acts like as an ultrasoft, multiphase material with distinct fluid and solid characteristics [3].

In a clinical setting, to relieve an elevated intracranial pressure, neurosurgeons remove part of the skull and allow the swollen brain to bulge outward [4]. This procedure is known as decompressive craniectomy and has been preformed for more than a century; however, its effects on the swollen brain remain poorly understood. Here we illustrate how to characterize the deformation, strain, and stretch in swelling brains using nonlinear finite element simulations [6]. For a personalized swelling simulation, we show that even small swelling volumes of 28 to 56 ml can induce maximum stretches on the order of 1.3, well beyond the safety limit. Our study suggests that the locations of maximum stretch and the associated failure modes of stretch and shear are universally shared amongst all swelling brains.

Modeling brain tissue as a multiphase material allows us to explain the mechanisms of swelling and make informed predictions about the accumulation of fluid in pathological conditions such as hydrocephalus or in response to traumatic brain injury. In combination with personalized simulations, multiphase modeling of the human brain tissue can guide surgical treatment planning with the ultimate goal to reduce brain damage and improve the structural and functional outcomes of neurosurgical procedures.

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Dynamic turnover of osteocyte pericellular matrix: Implications for osteocyte mechanosensing

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Nearly twenty years ago, Professor Stephen C. Cowin and his co-workers proposed that pericellular tethers surrounding osteocytes could serve as a mechanical means of strain amplification for osteocytes embedded in mineralized matrix to detect the small but critical mechanical strains that bone experiences in vivo [1]. A detailed mathematical model developed in 2001 demonstrated the feasibility of this novel hypothesis [2] and a 2004 transmission electronic microscopy study provided strong morphological evidence of such tethers [3]. Our collaborator, Professor M. C. Farach-Carson, identified perlecan (the large linear proteoglycan) within the osteocyte pericellular matrix in 2011 [4]. Our recent studies further demonstrated the critical roles of the osteocyte pericellular matrix on bone's responses to mechanical loading using a perlecan deficient mouse model, where we showed that the lack of perlecan nearly totally abolished the anabolic effects of mechanical loading on tibia seen in wildtype mice with normal expression of perlecan [5]. Interestingly, we recently discovered that just one day after a single session of mechanical loading, perlecan gene expression was upregulated even to a higher level than the genes encoding several matrix proteins such as collagen 1 and osteocalcin (3-fold vs. 1.5-fold, Fig. 1). This intriguing result suggests that the osteocyte pericellular matrix could undergo dynamic turnover, which has not been investigated yet. To this end, we adopted a newly developed metabolic labeling approach using modified sugars and click-chemistry labeling [6] to test (i) whether newly synthesized glycan-rich pericellular matrix of cultured osteocytes could be labeled, and (ii) whether mechanical stimulations impact the cells' synthesis of the pericellular matrix. After 24 hrs of feeding osteocyte-like cells (MLO-Y4) with modified sugars containing azide groups (Ac4GalNAz), a copper-free click chemistry reagent (DBCO-488) was applied to quickly label the surface glycans incorporating the modified sugars. Extensive green staining was seen around the cultured cells, which were labeled with a red-cell tracker (Fig. 2 Left) and multiple microvilli observed on the apical surface (Fig. 2 Right). Furthermore, we applied this metabolic labeling approach in vivo by injecting another modified sugar (Ac4ManNAz) for 7 days in B6 mice before DBCO-488 labeling. The newly synthesized matrix was clearly observed around osteocytes of tibial cortex under confocal microscopy (arrows in Fig. 3B). Ongoing efforts focus on how mechanical stimulation affects the production and turnover of the pericellular matrix in vitro and in vivo. The ultimate goal of this study is to understand the dynamics and biological functions of the osteocyte pericellular matrix, a critical component of mechanosensing in bone that was first proposed by Professor Cowin. This paper is dedicated to Professor Cowin, a great pioneer, scholar, and mentor.

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Effect of anisotropic microarchitecture on cancellous bone permeability and wall shear stress

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Fluid flow in the intertrabecular spaces of cancellous bone has been implicated in a number of physiological phenomena. According to Wolff's law of bone adaptation, interstitial fluid flow, driven by load induced gradients, is believed to be essential in the development of bone architecture and the bone's mechanosensory system by shearing bone cell membranes or causing cytoskeleton deformation [1, 2]. However, the relation between permeability and cancellous bone microarchitecture has not been fully investigated and few estimates of fluid velocities, pressures and wall shear stresses on the osteocyte process surface are available in the literature [3]. Experimental studies to quantify the mechanical environment surrounding bone cells are challenging, and as such, computational and theoretical approaches can be adopted to predict how these cells are stimulated in vivo. In this study we propose a framework to estimate the correlation between permeability, microarchitectural parameters (porosity, φ, trabecular thickness, Tb.Th, trabecular separation, Tb.Sp, connection density, Conn. D and the structural model index, SMI), fabric tensor, F and microvelocities in the intertrabecular pore space. Moreover, as a second objective, we computed the interstitial fluid velocity responsible for the wall shear stress on the lining cells. Computational Fluid Dynamic (CFD) simulations were implemented to compute the anisotropic permeability tensor in trabecular bone specimens based on micro computed tomography (CT) and artificial trabecular bone pores structures with increasing degree of anisotropy. Micro-CT images of human calcanei were obtained (13.5 µm resolution) and a 7x7 mm volume of interest (VOI) was numerically cropped from the center of the imaged sample. The subset of images was reoriented according to the principal fabric component and the intertrabecular space was segmented. Similarly, images of trabecular bone pores structures were obtained using Matlab 2014b (13.5 µm resolution). The model was imported into Abaqus 6.14-3. Microarchitectural parameters of both cancellous bone and trabecular pores structures were computed in CTAn software. Within the CFD software, boundary conditions were assigned to the model to replicate Darcy's law where a constant pressure differential across the specimen was maintained and the macro and microvelocities of the fluid measured [4]. Then the fixed wall condition necessary for the CFD analyses was removed to allow for the shear stress computation. The correlation of permeability and microarchitecture, F and microvelocities was fully investigated for trabecular bone pores structures with controlled geometry and tortuosity and human samples.

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Growth-Induced Stresses and Poroelastic Remodelling in Mechanotransduction of Solid Tumors

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Poromechanics plays a key role in modeling hard and soft tissue behaviors, by providing a thermodynamic framework in which different kinds of chemo-mechanical mutual interactions among heterogeneous fluid and solid constituents can be consistently rooted, at different scale levels [1]. In this context, the kinetics of interstitial tissue growth draws upon finite deformations and mixture-inspired models [2, 3] describing how the different biological species –including cells, extra-cellular constituents and chemical metabolites–exchange mass within complex open environments. Also, finite growth can be accompanied by the gradual change of the tissue properties and structural remodeling. Recently, attention has been focused on the biomechanical modeling of solid tumors seen as poroelastic masses cumulating residual stress during growth [4, 5]. Indeed, poroelasticity allows to highlight the key role of stresses and elevated interstitial fluid pressure (IFP) in influencing tumor development, demonstrating how intratumoral compression can both alter cells proliferation kinetics through specific mechanotransduction pathways and rule flow diversion and nutrients walkway towards the periphery of the tumor aggregates, in this way promoting cancer cells invasion and central hypoxia [6]. As a consequence, the prominence of the exact knowledge of the in vivo accumulated stress is strictly associated to the potential applications in cancer treatment, for example by designing ad hoc drug delivery strategies. However, how nonlinear elastic moduli depend on inelastic growth deformation, prestress and interstitial pore pressure is diriment to catch growth-induced stresses, both if one proceeds experimentally and through in silico simulations. To determine the explicit way in which the harboring stresses and stretches combine with the fluid pressure during growth processes is at the basis of tissue adaptation and material properties evolution, which in turn govern the growth fate. Therefore, we here provide a modeling approach to evaluate the actual updating of tangent moduli in nonlinear poroelastic growing (tumor) media, by investigating the direct correlation between the experimentally measurable tissue elastic constants and the in situ stress field, further including possible stress-induced heterogeneities and anisotropies, additionally discussing somehow unexpected possible local mechanical instabilities of the biological material.

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Interaction of ultrasound with cortical bone modeled as a two-level porous medium: a multiscale computational study

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Bone is a complex biological tissue which remodels all along healing. Bone remodeling is the result of bone cells activation due to mechanical stresses. The osteocytes are thought to be the principal mechanosensory cells of bone. They are immersed in the lacuno-canalicular network (LCN) filled with interstitial fluid. Theoretical and experimental evidences show that osteocytes are stimulated via shear flow acting on osteocyte cell processes within canaliculi. Low Intensity Pulsed UltraSound (LIPUS) is a current clinical treatment to speed up or consolidate bone healing. Although it has been proven that LIPUS induces minimal thermal effects, a debate is still opened to know how LIPUS mechanically stimulates bone regeneration. The aim of this preliminary study is to numerically investigate LIPUS stimulation from a tissue-scale model to a cellular-scale model in order to make the connection between in vitro studies and clinical observations. Two numerical models were developed by using the commercial software Comsol Multiphysics. The first tissue-scale model (ModBone) simulates the interaction of the ultrasound (US) stimulation with the cortical bone. Cortical bone is considered as a two-level-porosity medium: the vascular pores fulfilled by fluid are reconstructed from x-ray images and the lacuno-canalicular porosity is taken into account by assuming an anisotropic poroelastic extracellular matrix (ECM) (Cowin et al., 2009, Scheiner et al., 2015). The second model is the cellular-scale model (ModOst) including a 3D fluid-structure interaction model of one osteocyte immersed in the interstitial fluid of the LCN and embedded in the ECM. The pressure gradient induced by US stimulation in ModBone is applied as boundary condition for the fluid in ModOst. The interstitial fluid shear stress magnitude applied on osteocytes is calculated in the two models and compared with shear stress levels cell activation recorded in the literature (Weinbaum et al., 1994). How ultrasounds interact with bone tissue and which mechanical stimulation is induced on osteocytes remain tricky questions. Acoustic pressure and interstitial fluid pressure at tissue scale and wall shear stress on osteocyte are shown in the Figure. In this study, several points are still on going, among them: permeability value of the LCN, boundary conditions at the endosteum and periosteum, or the 3D reconstruction of vascular pore network.

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Modelling microbial processes in porous media under coupled flow, reaction and deformation phenomena

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Subsurface porous media, i.e., soils and rocks naturally contain copious amount of microorganisms. The presence of microbe, such as, bacteria and their microbial activity may significantly affect physical and chemical properties of the porous media as well as the local geochemical environment. Subsurface geological processes are often coupled in nature, involving multiple phases and geochemical reactions. Therefore, the study of microbial growth and consequent impacts on porous media under such condition is complex; difficult to mimic in laboratory and challenging to adopt in numerical models.

Within the scope of this study, a microbial model is developed under a coupled thermo-hydraulic-chemical-mechanical (THCM) framework. The aim of the model is to predict complex microbial growth and interaction processes, and assess the impacts on porous media both qualitatively and quantitatively. The coupled THCM model, namely, COMPASS is linked with the geochemical reaction model Phreeqc. This enables to model both equilibrium (i.e. speciation) and kinetically (i.e. mineral dissolution/ precipitation) controlled reactions occurring in subsurface geological formations.

In this presentation, developments of the model, including the important features are briefly detailed. Also, the applications of the model to predict biofilm growth in a multiphase system under the effect of local geochemical environment is presented.

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Poisson-Nernst-Planck-Fermi Theory for Biological Ion Channels

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A continuum-molecular theory --- Poisson-Nernst-Planck-Fermi theory --- has been developed in recent years for simulating ionic flows in biological ion channels under physiological or experimental conditions by treating ions and water of any size as non-uniform hard spheres with interstitial voids, polarization of water, and correlations of ions. The theory can also be used to study thermodynamic and electric properties of electrolyte solutions that are essential components in batteries, fuel cells, nanopores, porous media, geothermal brines, the oceanic system etc. The theory can compute electric and steric potentials from all atoms in a protein and all ions and water molecules in channel pore while keeping electrolyte solutions in the extra- and intracellular baths as a continuum dielectric medium. The PNPF model has been verified with the experimental data of L-type calcium channel, gramicidin A channel, and sodium/calcium exchanger with real structures from Protein Data Bank. It was also verified with the experimental or Monte Carlo data of electric double-layer capacitor and ion activities in aqueous electrolyte solutions.

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The velocity and attenuation of ultrasound wave in human cancellous bone is affected by charge density

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Poroelasticity is widely used for elucidating the bone fluid flow stimulating bone cells. These bone cells are communicating each other. The electrokinetic effect is another stimulus in bone remodeling process. The strain generated potentials (SGP) induce the charged ions flow through canalicular network. Excessive positive charge ions move along the bone fluid flow, which is called streaming potential. Two ultrasound waves are observed in cancellous bone. We show that the fast wave velocity and attenuation are affected by porosity as well as charge density in bone fluid flow, but, for the slow wave, both slow velocity and attenuation are not sensitively affected by charge density in bone fluid flow. Thus we conclude that the charge ions are gathered on the trabecular struts and the fast wave, which moves along the trabecular struts, is affected by charge density, after employing human femoral data into governing poroelasticity equations. We definitely need further experiments to examine the charge ion effect on trabecular struts, but it is difficult in setting up the experiment. Thus we will combine the piezoelectric effect, which is another bone remodeling stimulus, into poroelasticity governing equation and we will make experimental setup possible for future experiments.