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Book of abstracts of International Conference on Porous Media (InterPore)

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International Society for Porous Media

Book of abstracts of International Conference on Porous Media

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Since its foundation in 1995 the Fraunhofer ITWM, the Institute for Industrial Mathematics, has shown great success in building mathematical bridges between applied sciences and concrete application. Clients are large international companies as well as small and medium regional enterprises. Fraunhofer ITWM focuses on the development of mathematical applications for industry, technology and economy. Mathematical approaches to practical challenges are the specific competences of the institute and complement knowledge in engineering and economics in an optimal way. In 2001 ITWM became the first mathematical oriented institute of the Fraunhofer Society. The main emphases are surface quality inspection, financial mathematics, visualization of large data sets, optimization of production processes, virtual material design and porous and composite material simulation.

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Computer simulations are an indispensable tool in the design and optimization of products and production processes, services, communication processes and work processes. Real models are replaced by virtual models. Mathematics plays a fundamental role in the creation of this virtual world. Mathematical models cut horizontally across a landscape of vertically arranged scientific disciplines and technological applications. This transverse character of mathematics makes it a “generic technology”; as a basis for bridging into the simulation world, however, it also becomes the key technology for computer simulations which have found their way into nearly all areas of economic life. Increasingly more small and medium-sized companies utilise simulation for cost reduction. It is specifically these companies that the Fraunhofer ITWM supports with consultation and computing power. They profit in the market through the use of simulation as identification for innovation and quality assurance of their products.

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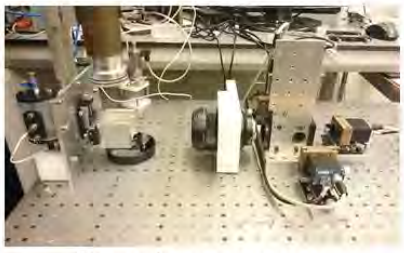
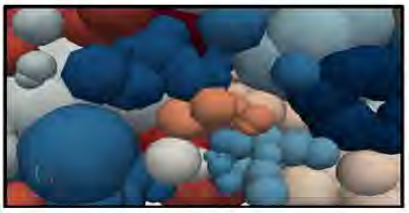
- Visualization of flow of immiscible fluids and motion of nano- and micron-sized particles in nano and micro-structures, and 3-D imaging of porous structures such as paper, fuel cell layers and beds of swelling particles using our **Confocal Laser Microscope**.
- Visualization of flow of immiscible fluids and solute transport in microstructures using an **open microscope setup** designed and developed in our own laboratory.
- Noninvasive measurement of soil moisture and saturation of fluids using our state-of-the-art **dual energy gamma system** in sand boxes and soil columns.
- Characterization of hydraulic properties of soil and porous structures using in-house made setups, Hydroprop, and pore-scale models
- We have a rich collections of in-house developed software packages, which can perform virtual experiments using our complex **pore-network models** and **grain-scale models**.
- Experience in the application of models used in fluid-dynamics and porous media

Nikon A1R confocal microscope

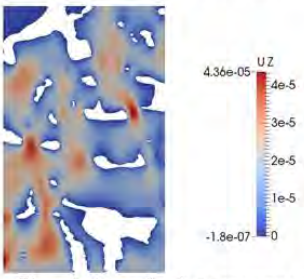


Open microscope set-up

Gamma ray system



Simulated bed of AGM particles



Simulation of solute transport

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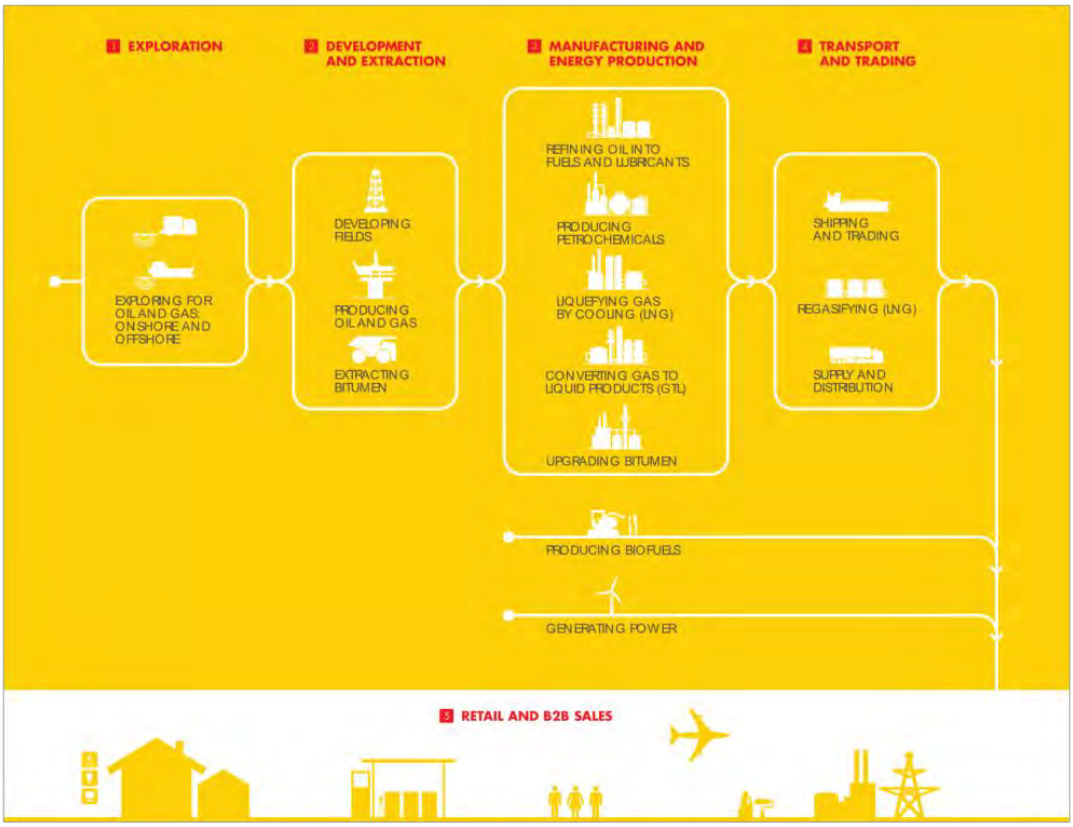

UPSTREAM 2014 HIGHLIGHTS

- 3.1 million boe/ d production
- 24.0 million tonnes of LNG sold
- $15.8 billion earnings
- $31.8 billion cash flow operations
- 10 frontier and heartlands discoveries and successful appraisals
- 3 final investment decisions on key projects
- 4 production start-ups of operated deep-water projects

Upstream explores for and recovers crude oil, natural gas and natural gas liquids, liquefies and transports gas, and operates the upstream and midstream infrastructure necessary to deliver oil and gas to market. Upstream is managed in two businesses: Upstream International and Upstream Americas.

DOWNSTREAM 2014 HIGHLIGHTS

- 6.4 million b/ d oil products
- $ 3.4 billion CCS earnings
- $ 11.3 billion cash flow from operations
- 43 thousand branded retail sites in more than 70 countries
- 85% chemical plant and highest ever refinery availability during a year, 94%

Downstream manages Shell's refining and marketing activities for oil products and chemicals. These activities are organised into globally managed classes of business, although some are managed regionally or provided through support units.

PROJECTS & TECHNOLOGY KEY STRENGTHS

- Innovation and R&D
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- Project execution

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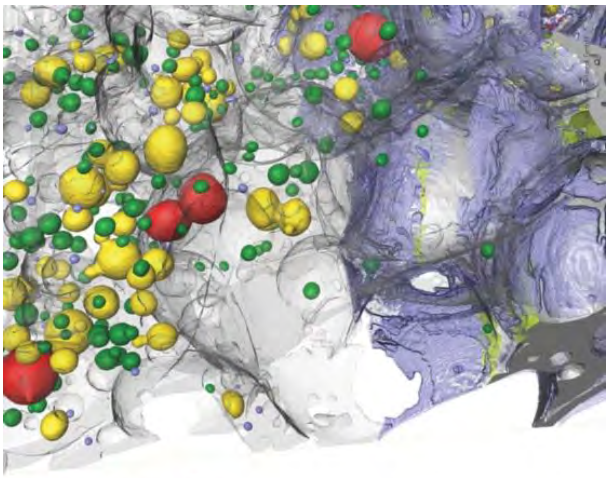

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- **Nikhil Palakurthi**, UC Simulation Center

Plenary speakers

Invited speakers

Minisymposium 1.1 - Mixing and reaction in permeable media from pore to continuum scale

Minisymposium 1.2 - Fundamentals of enhanced oil recovery: experimental and modelling techniques

Minisymposium 1.3 - Vapor transport through and phase changes within partially saturated porous media

Minisymposium 1.4 - Fluids in nanoporous media

Minisymposium 1.6 - Improved oil recovery by low salinity waterflooding – consistency through the scales

Minisymposium 1.7 - Modelling interfaces between porous media and free fluids

Minisymposium 1.8 - Porous electrode theory for rechargeable battery materials: state of the art, limitations, and opportunities

Minisymposium 1.9 - Minisymposium in honor of Geoffrey Mason

Minisymposium 1.10 - Mechanics of unsaturated porous media: the interplay of phases and interfaces in various phenomena

Minisymposium 1.11 - Non-Newtonian flow in porous media

Minisymposium 1.12 - Simulation (lab, virtual) as a source of new knowledge

Minisymposium 1.13 - Upscaling for complex flows in porous media

Minisymposium 1.14 - Challenges in modeling and characterization of transport in low permeable media

Minisymposium 2.1 - Pore-scale simulation and upscaling technology in unconventional oil/gas reservoirs

Minisymposium 2.2 - Pore-scale modeling and experiments on multiphase flow in porous media

Minisymposium 2.3 - Contact-line dynamics in pore scale modelling: from the diffuse interface to the sharp limit

Minisymposium 2.4 - Modeling and simulation of nanoparticles transport in porous media

Minisymposium 2.5 - Reconstruction of disordered porous materials and media

Minisymposium 2.6 - Multiscale model reduction techniques for porous media processes

Minisymposium 2.7 - Uncertainty quantification in porous media simulations

Minisymposium 2.9 - Novel discretization techniques for multiphase flow and transport in porous media

Minisymposium 2.10 - Advanced numerical methods for subsurface flow simulations in poro-fractured media

Minisymposium 2.11 - Transport characterization of coupled multi-physics phenomena in porous media

Minisymposium 2.12 - Imaging, characterization and modeling of flow and deformation in fractured porous media

Minisymposium 2.14 - Integration of data and modeling from multiple scales

Minisymposium 2.17 - Experimental and computational challenges in fuel cells and electrochemical devices

Minisymposium 2.18 - Porous media and filtration

Minisymposium 2.19 - Advances in the simulation, prediction, measurement, or upscaling of chemical reactions from pore- to field-scale

Minisymposium 3.1 - Application of magnetic resonance imaging (MRI) to porous media

Minisymposium 3.2 - Porous micromodels: advances in microscopic and macroscopic methodologies

Minisymposium 3.3 - Microscale approaches to close, evaluate, and validate emerging multiscale theories

Minisymposium 3.5 - Transient methods to identify effective parameters in porous media

Minisymposium 3.6 - Porous materials in biotechnology

Minisymposium 4.1 - Foam transport through permeable media: Fundamentals and applications

Minisymposium 4.2 - Thin porous media

Minisymposium 4.4 - Paper-fluid interactions: experimental studies and modeling

Minisymposium 4.5 - Multiphase flow and reactive transport at the pore scale: direct comparison of experiments and numerical simulations

Minisymposium 4.7 - Porous media evolving: mechanism, theory and applications

Minisymposium 4.10 - Multiscale transport processes in biological tissues

Minisymposium 4.12 - Transport of living/active particles in porous media: from the micro-hydrodynamic scale up to the Darcy scale

Minisymposium 4.14 - Coupling of flow and deformation in swelling porous materials

Minisymposium 4.15 - Transport in construction and building materials under environmental loading

Minisymposium 4.16 - Flow batteries

Minisymposium 4.19 - Wood as a porous building material

Minisymposium 4.20 - Anomalous diffusion in porous media

Minisymposium 4.23 - Flow and transport over porous media

General Session 1 - General session on fundamentals of porous media

General Session 2 - General session on computational challenges in porous media simulation

General Session 3 - General session on experimental achievements

General Session 4 - Other topics related to porous media

Special Session - Complex dynamics of drying in porous media: Linking experimental and modelling observations

From biofilms to diffusiophoresis: New observations about transport processes in porous media

Presenter: Howard Stone
Contact Author: Howard Stone

AUTHORS

Howard Stone [1]

1 Princeton University, MAE, 1 Olden Street, 08544, Princeton, US

ABSTRACT

We describe two distinct flow environments that influence particle-related transport in porous materials. First we consider biological transport problems associated with bacteria and biofilms. To begin, we consider the movement of surface-attached bacteria that can be motile on substrates. We document that in a channel flow the bacteria can migrate upstream, opposite the direction of mean flow, and we characterize how the dynamics enhance spreading in a porous system. The bacteria can form biofilms and so we then document how biofilms, which are a form of soft material, can form three-dimensional filaments inside flow channels and develop to cause catastrophic clogging. Also, we highlight how the chemical signalling known as quorum sensing is influenced by flow in confined spaces and show that, under flow, genetically identical cells do not exhibit phenotypic uniformity with respect to quorum sensing in space and time, leading to
complex patterns of pathogenesis and colonization. In a separate line of work we consider diffusiophoresis, which refers to particle transport driven by chemical gradients. Specifically we describe the control of diffusiophoretic transport in porous systems, including those with dead-end pores.

Pore-scale studies of multiphase fluid flow in porous media

Presenter: D.A. Weitz
Contact Author: D. A. Weitz

AUTHORS

D. A. Weitz[1]

[1] Dept. of Physics and SEAS, Harvard University, Cambridge MA 02138

ABSTRACT

This talk will describe studies of multiphase flow in porous media using a micromodel system in which both phases are index-matched to the porous media, enabling confocal microscopy to be used to image the flow of both fluids in three dimensions. The fluid flow is measured at the pore scale using both imaging to determine the location of the fluids, and PIV (particle imaging velocimetry) to determine spatial maps of the fluid flow lines within the pores. The results provide new insight into the nature of the flow and the role of polymer during polymer floods.

Nanostructured Materials for Application in Electrochemical and Chemical Energy Storage

Presenter: Sarah Tolbert
Contact Author: Sarah Tolbert

AUTHORS

Sarah Tolbert [1]

1 Departments of Chemistry and Biochemistry, Materials Science and Engineering, and the California NanoSystems Institute, UCLA, Los Angeles, US

ABSTRACT

In this talk, we examine ways that solution processed nanostructured materials can be used to address issues of relevance to energy storage and harvesting. We begin with work on nanoporous materials for electrochemical energy storage. Materials with appropriate nanoporous architectures can be synthesized using either block-copolymer templating methods or using selective solution phase dealloying of mixed metal solid-state precursors. The resulting nanoporous materials can form the basis for high power electrochemical energy storage materials known as pseudocapacitors. In such materials, the nanoscale porosity can produce a very desirable combination of electrical connectivity, electrolyte access to the interior of the material, ample surface redox sites, and very short solid-state diffusion lengths for lithium ions. With idealized architectures, we have shown that a unique combination of high energy density and high power density can be achieved, in some case combined with reactivity toward ions other than Li+. Moreover, by combining structural and electrochemical measurements on a range of materials, we can begin to determine design rules for the fabrication of next generation porous electrode materials. We will next examine chemical energy storage in the form of electro-catalytic water splitting. Here we again utilize nanoporous materials made by dealloying. We specifically examine porous metal/metal oxide NiFe based materials as efficient catalysts for the water splitting oxygen evolution reaction. Taken together, the results show how controlled nanoscale architecture has exciting potential to impact the global energy problem.

Ten Principles of Innovation

Presenter: Paul Trokhan
Contact Author: Paul Trokhan

AUTHORS

Paul Trokhan [1]

1 Senior Innovator-VMS Upstream Development Engineer in the Tissue/Towel Global Business Unit of Procter and Gamble, Procter and Gamble Company (P&G), US

ABSTRACT

Virtually all businesses set stretching growth goals. While the strategies on how to achieve those goals vary greatly, one underlying theme remains constant: game-changing innovation at all levels and across all functions and disciplines is essential. While there are no prescriptive checklists that guarantee success, efforts driven by personally derived innovation principles increase the probability that meaningful advances will occur. Every individual in the organization should be encouraged to develop such principles and then routinely exhibit what I call constructively deviant behavior. This talk outlines ten fundamental principles that have guided my 37 years of upstream R&D work at Procter & Gamble. The principles touch on forgetting a lot of what you have been taught, being a beta risk minimizer and fostering the right attitude to be successful in a large corporate culture.

Cryogenic Broad-Ion-Beam milling and Wood's-Metal-Injection: two new techniques required to better understand fluid distribution and effective porosity in porous and sensitive materials using a Scanning Electron Microscope

Presenter: Joyce Schmatz
Contact Author: Joyce Schmatz

AUTHORS

Joyce Schmatz [1], Jop Klaver [2], Janos L. Urai [3]

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3 Structural Geology, Tectonics,and Geomechanics, RWTH Aachen University, Lochnerstrasse 4-20, 52056, Aachen, DE

ABSTRACT

Pore geometries and associated mineral phases and fluids are important properties in fine-grained rocks such as cap rocks (e.g., chalks, mudstones and shales) or reservoir rocks (e.g., gas shales, tight gas sandstone and carbonates). Imaging of the pore space on Broad Ion Beam (BIB) polished cross sections in the Scanning Electron Microscope (SEM) allows accurate quantification of the pore characteristics from milli- to nanometer-scale resolution on a relatively large area, as shown over the past few years in numerous applied studies (Hemes et al., 2015; Houben et al., 2013; Klaver et al., 2015). We obtain the mineral porosity by combining image data from SE, BSE and EDX detectors using dedicated image segmentation algorithms, which automate the process of porosity analysis. Our workflow allows for accurate segmentation of pores and determination of phase porosity so that pore statistics and physical properties of the materials, such as pore size distribution and permeability, can be inferred. It was found that the visible pore size distribution, e.g., in fine-grained rocks, follows a power-law behavior from the micrometer down to the nanometer range (Houben et al., 2013).
Recent developments of the technique allow studying the in-situ fluid distribution in wet rocks: BIB-SEM under cryogenic conditions was used to quench a range of rock types to liquid nitrogen temperature: mudstones, evaporites (Desbois et al., 2013), and also the oil-water-mineral system in hydrocarbon-bearing reservoirs (Fig. 1, Schmatz et al., 2015). Subsequently they were cut with a saw under cryogenic conditions and subsequently sectioned using cryo-BIB-milling. The flat cross-sections with dimensions of 4 mm2 allow cryo-SEM imaging of oil-brine-mineral interfaces, with high-resolution EDX-mapping for phase identification. 3D-reconstruction of capillary contact angles was done using serial sectioning with a distance of 1 µm. Sub-micron effects on fluid flow, such as rugosity effects or thin water films separating the hydrophilic mineral surface from the oil, can be revealed with this technique, which however cannot be obtained by e.g., Micro-CT. Such significant results call for improvements in models of multiphase pore-scale flow in digital rocks. Further anticipated applications of the method are e. g., the investigation of pore-level mechanisms of Enhanced Oil Recovery (EOR) or aging processes; the investigation of oil-sands, gas-hydrates, and other sensitive or wet materials; or the investigation of in-situ fluid distribution reservoir- sandstones and carbonates.
Combining BIB-SEM with Wood's Metal Injection (WMI) enables to quantify pore connectivity, to determine the controlling pore throat diameter, and visualizing the preferred transport pathways. The technique resembles mercury intrusion porosimetry with the great difference that we can image which parts of the sample were intruded by the low temperature fusible alloy. The WMI experiments illustrated the significant effect of fractures on transport pathways and the low connectivity of the

clay-rich matrix in mudstones (Klaver et al. 2015). Additionally, the method allowed for determination of e.g., the effect of mineralogy on the pore connectivity, shown in preferred streamline pathways through distinct phases, while other phases of similar porosities were not percolated (Fig. 2).

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Reduced-order models for optimization of subsurface flow processes

Presenter: Louis Durlofsky
Contact Author: Louis Durlofsky

AUTHORS

Louis Durlofsky [1]

1 Stanford University, Green Earth Sciences Bldg, 94305-2220, Stanford, US

ABSTRACT

Reduced-order models (ROMs) are well suited for use in applications that require large numbers of related simulations, such as optimization and uncertainty quantification. In this talk, reduced-order modeling procedures applicable for simulating oil recovery processes and geological carbon storage operations will be developed and applied. The ROMs considered entail the representation of new solutions as expansions around previously-simulated 'training' solutions. A method based on linear expansions (trajectory piecewise linear, TPWL) will be described, as will a new approach that includes higher-order terms (trajectory piecewise quadratic, TPWQ). By projecting these representations into a low-dimensional subspace using proper orthogonal decomposition (POD), we arrive at highly efficient (in terms of runtime) POD-TPWL and POD-TPWQ procedures. The use of these ROMs for simulating and optimizing geological carbon storage and oil recovery processes will be demonstrated.

Experimental imaging and upscaling of mixing and reaction processes in porous media

Presenter: Tanguy Le Borgne
Contact Author: Tanguy Le Borgne

AUTHORS

Tanguy Le Borgne [1], Pietro de Anna [2], Joaquin Jimenez-Martinez [3], Regis Turuban [4], Aditya Bandopadhyay [5], Hervé Tabuteau [6], Yves Méheust [7], Tim Ginn [8], Daniel Lester [9], Marco Dentz [10], Emmanuel Villermaux [11]

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9 Royal Melbourne Institute of Technology, Melbourne, AT
10 CSIC Barcelona, Barcelona, ES
11 Aix-Marseille University, Marseille, FR

ABSTRACT

Fluid mixing processes play an important role to trigger reactions in porous media, including dissolution and precipitation in CO2 sequestration operations, biochemical clogging in geothermal dipoles, biofilm growth in oxidation-reduction fronts, and reaction enhancement in flow-through reactors. The broad distributions of velocities inherent to porous media flows can either enhance effective reaction rates by bringing reactants into contact or reduce them by inducing a spatial segregation of chemical species. How to relate structural porous media heterogeneities and complex flow topologies to effective mixing and reaction rates is a currently open question that is common to a large spectrum of reactive transport processes in porous media.

This presentation will discuss this issue in the light of recently obtained millifluidic experimental datasets that exploit fluorescence and chemiluminescent imaging techniques to quantify two-dimensional distributions of concentrations and reaction rates at pore scale. Using these techniques, the interplay between broad velocity distributions, dispersion, mixing and chemical reactions is documented for different structural heterogeneities, flow rates and initial conditions in both saturated conditions and multiphase flows. High resolution pore scale images of concentration and reaction rate distribution show the formation of well-developed filamentary structures in reactive mixtures transported through porous media (de Anna et al. EST 2014). These elongated lamellar patterns, naturally created by the stretching action of the pore scale velocity field, are shown to affect mixing and chemical reactions over orders of magnitude (de Anna et al. GRL 2014, Le Borgne et al. GRL 2015, Jimenez-Martinez et al. GRL 2015). Hotspots of mixing and chemical reactions are found to be located in the area with largest velocity gradients that induce large fluid stretching rates. At late times or at low Peclet numbers lamellar patterns are no longer visible since they have been merged by diffusive aggregation. However, they still control concentration distributions that evolve towards uniformity via a continuous self-aggregation process (Le Borgne et al. PRL 2013). In this regime, the highest concentrations are found in the areas where lamella aggregation rates are largest. The distribution of concentrations and reaction rates can be related to the frequency of lamella diffusive overlap through generalized random aggregation equations (Le Borgne et al. JFM 2015).

Understanding mixing as a lamella stretching and aggregation process provides a new theoretical

framework for quantifying concentration distributions and effective reaction rates in porous media. Based on this theory, we derive analytical predictions for the probability density functions of concentration values, concentration gradients and chemical reaction rates (Le Borgne et al., PRL 2013, Le Borgne et al., JFM 2015). The obtained theoretical predictions and upscaled effective mixing and reaction kinetics are in good agreement with experimental and numerical results at both pore scale and Darcy scale, over a broad range of time scales, Peclet and Damköhler numbers and for different degrees of heterogeneity. We generalize these results for different type of random flows, including porous media and turbulent flows, and discuss perspectives for upscaling mixing and reactive transport in different applications.

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Multi-scale Modeling and Simulation of Composite Manufacturing Processes

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ABSTRACT

This talk will focus on how the science base of materials processing, which integrates material parameters with transport phenomena at various scales during manufacturing, can be used to create multi-physics models and implemented in simulations to describe the effect of material, geometric and process parameters on the final quality of the composite part. The simulations are tailored to address resin flow in Liquid Composite Molding processes such as Resin Transfer Molding, Vacuum Assisted Resin Transfer Molding and Compression Resin Transfer Molding. In such processes, the fiber preform is placed in a closed mold and resin is injected from injection gates to cover all the empty spaces between the fibers. The injection gates are closed when the resin reaches the vent hole displacing the air out of the mold. The part is de-molded once the resin cures. The goal of the simulation is to optimize the gate and vent locations to ensure that no air pockets or fibers not covered by resin exist within the part. The fiber preform is a dual scale porous structure with fiber tows woven or stitched together to form a textile. Each tow is of the order of millimeters and consists of three to twelve thousand continuous aligned fibers of micron size diameter bundled together. Examples of flow simulations in the dual scale pores will be discussed with experimental validation and their relevance in composite manufacturing will be highlighted.

Electrospinning of Porous Fiber Membranes and Their Applications

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ABSTRACT

Electrospinning utilizes a voltage to induce sufficient charges in a polymer solution to overcome the surface tension of the liquid and force a fluid jet to be ejected. The liquid jet undergoes simultaneous whipping and evaporation resulting in a solid polymer fiber. This straightforward technique has produced micro-/nano-fibers from a large variety of polymers. Key features of the fiber electrospinning process include: (a) control of the fiber diameter from micro- to nano-meter dimensions; (b) production of very long fibers (cm-km); (c) control over the fiber compositions; (d) spatial alignment of multiple fibers. The resulting fiber membranes have a non-woven porous structure with very high surface-to-volume ratio. These membranes are fully formed during the electrospinning process and, thus, do not require a drying step, high temperatures or pressures. This makes them particularly attractive for the incorporation of labile biomaterials.

An overview of the fiber electrospinning process is first presented. The key significant parameters are identified and briefly discussed: external electric field, polymer solvents/solubility, solution electrical conductivity, viscosity, and surface tension. Next, coaxial electrospinning is introduced. This advanced technique greatly expands the capability of electrospinning by enabling the formation of core-sheath fibers in a single step. This is accomplished by feeding two separate polymer solutions through a coaxial nozzle that consists of a central tube surrounded by a concentric annular tube. This core-sheath concept is extremely versatile, as it can combine different properties from core and sheath materials into a single fiber. Compared to alternative methods for core-sheath fiber production, coaxial electrospinning provides a simple, one step and highly cost-effective process. It can utilize a large variety of materials and controllable thickness of core-sheath structured fibers, without the need for vacuum, elevated temperature treatment, plasma exposure or sophisticated chemistry. The requirements for successful coaxial electrospinning are identified, including viscoelastic properties, immiscibility and inter-diffusion, dielectric constants, evaporation rates, solution feeding ratio, etc.

Applications of uniform and coaxial electrospun fibers are briefly reviewed: tissue engineering, controlled drug delivery, superhydrophobic membranes, encapsulation of biopolymers or fluids, micro/nanofluidic devices, textile applications, self-cleaning fibers. Finally, tri-layer core/intermediate/sheath (“triaxial”) fibers and their applications are introduced.

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Representation of reactive interfaces in direct numerical simulation of pore scale processes

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ABSTRACT

Reactive processes in porous media such as mineral dissolution-precipitation take place at interfaces between fluid and solid phases. Because the different phases are distinguishable at the pore scale, experimental and modeling studies need to consider these interfaces to accurately determine reaction rates [1]. Direct numerical simulation (DNS) of pore scale processes entails the use of conventional discretization methods to solve the flow, transport and geochemical equations with an explicit representation of the reactive interfaces.

In this presentation, we summarize the development and application of a new generation of pore-scale flow and reactive transport models based on a DNS approach [2, 3]. In the simulations, the incompressible Navier-Stokes equations are solved together with the multicomponent reactive transport equations for the chemical system. A Cartesian grid embedded boundary method, whereby interfacial surfaces were described by a cut-cell approach, was used to directly account for the surface area available for reaction—rather than treating reactive surface area as a continuum-scale parameter. Further, an adaptive mesh refinement algorithm is used to provide additional resolution near reactive surface for increased accuracy. A conservative embedded boundary method was also developed for time dependent domains [4], such as those where dissolution-precipitation changes the geometries of mineral surfaces.

The model is used to explore the impact of pore scale flow on the reaction rates. More specifically, it is used to evaluate the relative importance of transport processes on controlling dissolution rates [2-3], including the development of diffusive boundary layers [5], and in turn, in shaping the textural evolution of porous media.

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Multiscale reservoir simulation: From Poisson's equation to industry-standard models

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ABSTRACT

A wide variety of multiscale methods have been proposed in the literature to reduce runtime and provide better scaling for the solution of Poisson-type equations modelling flow in porous media [1]. The key idea of all these methods is to construct a set of prolongation operators (also called basis functions) that map between unknowns associated with cells in a fine-scale geological reservoir model and unknowns on a coarser grid used for dynamic simulation. The prolongation operators are computed numerically by solving localized flow problems, much in the same way as in flow-based upscaling methods. The prolongation operators are then combined with a suitable restriction operator to construct a reduced coarse-scale system of flow equations that describe the macro-scale displacement driven by global forces. Unlike effective parameters, multiscale basis functions have sub-scale resolution, which ensures that fine-scale heterogeneity is correctly accounted for in a systematic manner and enables us to reconstruct an approximate fine-scale solution once the global coarse-scale system is inverted.

For the past ten years or so, my research group has worked on adapting and extending these methods so that they can be applied to simulate real petroleum reservoirs. In the first part of the talk, I will briefly explain why this is a difficult undertaking, review key ideas that have been researched, and point out failures and successes.

In the second part of the talk, I discuss what is currently the most versatile and robust multiscale formulation, the multiscale restriction-smoothed basis (MsRSB) method [2]. This method has been implemented in the prototyping branch of a commercial simulator and has three main advantages: First, the input grid and its coarse partition can have general polyhedral geometry and unstructured topology. Secondly, MsRSB is accurate and very robust compared to existing multiscale methods. Finally, the method is formulated on top of a cell-centred, conservative, finite-volume method and is applicable to any flow model for which one can isolate a pressure equation. I end the talk by discussing several examples, including 3-phase black-oil models, polymer flooding with non-Newton fluid rheology, and embedded fracture models.

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Transport of cryoprotectants in articular cartilage: How math can save knees

Presenter: Janet A. W. Elliott
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ABSTRACT

Cryobiology is the study of life at low temperatures with a major application being preservation of cells and tissues for medical transplantation. A favored approach in the cryopreservation of tissues is the use of up to 50% by weight cryoprotectants to avoid ice formation upon cooling to liquid nitrogen temperatures (–196 °C), i.e. vitrification. The problem of successful vitrification of tissues is how to load a vitrifiable amount of cryoprotectants before the toxicity limits of cells are reached. Articular cartilage is the smooth white substance covering the ends of bones to allow joints to articulate. It is the tissue that is diseased in osteoarthritis and has been transplanted with success in cases of major joint defects. In collaborative research spanning 15 years, we combined mathematical modelling with biological experiments to develop the first successful protocol to cryopreserve intact human articular cartilage on bone with high cell viability and function. A key component of this work was modeling and optimizing the diffusion of cryoprotectants in cartilage. This presentation will describe our model of the transport of thermodynamically non-dilute amounts of cryoprotectant in the linear elastic porous medium of cartilage including water movement, the role of ions, and the spatially varying tissue shrinking and swelling [2–4]. The model was verified by comparison to novel spatially and temporally resolved spectral magnetic resonance imaging measurements [4]. This research was funded by the Canadian Institutes of Health Research (CIHR) and the Natural Sciences and Engineering Research Council (NSERC) of Canada. J. A. W. Elliott holds a Canada Research Chair in Thermodynamics.

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Porous media from self-assembly and their applications

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ABSTRACT

Porous materials providing well defined pore sizes and pore structures combined with large surface areas are important for a number of applications ranging from separation and catalysis all the way to energy conversion and storage. In this talk the formation of porous materials will be discussed on the basis of block copolymer self-assembly. The emphasis will be on the development of wet chemical methodologies towards the control of size, structure, and order of porous materials based on an understanding of the fundamental principles that govern structure formation. This will cover systems at or close to the thermodynamic equilibrium as well as approaches where systems are systematically driven away from equilibrium to achieve structure control otherwise impossible. Examples will include isoporous block copolymer-based membranes for ultrafiltration applications with graded pore structures, hierarchical porous polymer scaffolds from a combination of spinodal decomposition and microphase separation in block copolymer-organic additive mixtures, shape control of hierarchical porous all-organic thin films via transient laser heating and their conversion into 3D periodic mesoporous semiconductors, as well as the first report on block copolymer self-assembly based mesoporous gyroidal superconductors.

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Mixing Across Scales in Heterogeneous Media: From Physical Non-Equilibrium to Anomalous Chemical Transport

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ABSTRACT

We consider phenomena of transport and reaction in heterogeneous porous media from a mixing perspective. Anomalous or non-Fickian transport and reaction phenomena, this means, behaviors that cannot be described by advection-dispersion-reaction equations characterized by equivalent transport and reaction parameters, can be linked to incomplete mixing or physical non-equilibrium. We first review the signatures of physical equilibrium in terms of Lagrangian and Eulerian transport frameworks and its breakdown in the presence of spatial heterogeneity. We discuss the manifestations of incomplete mixing in terms of characteristic scales and Lagrangian particle transitions. This leads us to alternative non-equilibrium transport frameworks in terms of the continuous time random walk. We discuss this approach as an upscaling framework for transport and chemical reactions from pore to Darcy to field scale based on experimental, numerical and theoretical arguments. We illustrate the impact of incomplete mixing and reactant segregation on large scale reaction dynamics for both mixing as well as kinetics limited chemical reaction and provide a direct link to anomalous transport characteristics.

Membraneless Flow Batteries and Desalination: Ion Transport in Cross Flow in Porous Media

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ABSTRACT

Flow batteries, fuel cells, electrolyzers, and desalination systems typically employ open flow channels separated by ion-exchange membranes. This talk describes two examples of "membraneless" electrochemical cells exploiting cross flow in porous media, either to keep reactants apart (membraneless flow battery) or to achieve charge-based separations (shock electrodialysis). In the first case (Fig. 1), a porous dispersion blocker between porous flow-through electrodes enables closed-loop cycling of a hydrogen-bromine flow battery, thus potentially lowering cost and increasing lifetime and power density by eliminating the need for a cation-exchange membrane [1]. In the second case (Fig. 2), a charged porous medium acts as a "leaky membrane" to sustain a deionization shock wave during the passage of over-limiting current, which can be used to continuously deionize and disinfect water in cross flow [2,3]. Heterogeneous, hierarchical and anisotropic porous media could lead to further breakthroughs in these novel flow-through electrochemical systems.

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Fast Solvers for Coupled PDE problems with Applications in Porous Media Science

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ABSTRACT

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 often also 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 take an application oriented approach, and focus on the problem classes of poroelasticity problems and density-driven-flow. For these two examples, we outline a common solution strategy, and provide numerical results.

Self-sealing or self-enhancing? Observations of fracture evolution during CO2 induced dissolution at in-situ conditions using synchrotron microtomography

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ABSTRACT

The long-term security of sequestered CO2 is dictated partially by the integrity of sealing formations, typically shales, tight carbonates, or anhydrites. At present, the permeability evolution of flaws in such seals (e.g. fractures and faults) when exposed to streams of either scCO2 or carbonated brines is not well understood; this is due to the complex coupling between reactions, flow, and in-situ stress conditions. A key open problem is the long-term evolution of fracture aperture (and therefore permeability) for induced fractures in low permeability carbonates, a process which can control seal integrity at sites being utilized for CO2 storage. Experimental and field evidence exist for both self-sealing and self-enhancing reactive alterations during flow of CO2 charged brines through tight formations, likely controlled by a host of hydrological, geochemical, and geomechanical variables.

We present results from a series of dynamic synchrotron X-ray microtomography (SXR-?CT) experiment investigating changes in fracture aperture during dissolution induced by CO2 saturated water. The samples explored include a low-permeability dolomite from the Duperow formation and a carbonate rich shale from the Niobrara unit. Both experiments were conducted near in-situ conditions using an x-ray compatible triaxial pressure vessel. Results show distinct fracture evolutions pathways for the two samples due to the microstructure of the non-reactive phase in both cases. Both experiments also revealed a strong feedback between reaction rates in the reactive and non-reactive mineral phases during dissolution and the development of a pronounced high-porosity weathered zone in the near-fracture region. Surface roughening and fines mobilization were also observed during dissolution. Confining stress cycles conducted after initial flow confirmed that the asperities remained strong even after exposure to aqueous CO2 for prolonged periods.

On-going modeling studies using both fracture scale and continuum reactive transport models should assist generalization of these observations to assist in selection of seals with higher likelihood of resilience after fracturing or fault reactivation.

Scaling relationships for vegetation and soil development: from seconds to millennia and beyond

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ABSTRACT

Flow and transport in heterogeneous porous media with distributed local conductance values is best treated using concepts from percolation theory. A theoretical treatment of solute transport in porous media1-3 combines critical path analysis and cluster statistics of percolation theory to generate the probability that a spanning cluster with a given minimum resistance value is found; the transport time across such a cluster is given by scaling arguments from percolation theory. This theoretical treatment has been shown to generate solute arrival time distributions as functions of saturation in agreement with predictions3 and to predict the scaling of silicate weathering and other reactions, both in situ and in the laboratory, over time scales from hours to almost 10 million years4. Thus, the scaling of the solute fluxes matches the scaling of the reaction rates, implying that, under most or all circumstances, reactions are transport-limited. Consequently, the reaction front (the weathered soil horizon) should have advanced a distance equal to the transport. In a simple scaling argument from percolation theory the transport time is proportional to the distance to a power equal to the fractal dimension of the percolation backbone in three dimensions (1.87), approximately valid whenever flow properties could be calculated using critical path analysis5, turns out to be sufficient to predict soil formation depths at time scales up to 100 million years, and soil production functions to 30 million years. The solute transport velocity, equal to that of the fluid at the scale of a single pore, diminishes approximately according to a power law at larger spatial scales. The topology of solute transport paths in random porous media is such that the time for solutes from microscopic sources to be transported up to 100 meters can be 100 million years, but dendritic root structures allow plants to access nutrients much more rapidly, since the relevant exponent relating space and time is now only that of the optimal paths in two dimensions, which replaces the exponent 1.87 by 1.21. Maximum growth rates of intensively managed vegetation, owing to the lack of nutrient limitation, are equal to the typical flow rate in the subsurface. Confirmation of the validity of these scaling relationships is demonstrated by comparison with hundreds of sources of plant growth data, and over fifty sources of soil depth and soil production. Simultaneously, it is shown that soil C and N sequestration rates are proportional to soil production and chemical weathering rates, as predicted when soil weathering is solute transport limited. The second order effect is shown to be flow rate variability, as predicted in the scaling relationship. Thus, carbon sequestration through 1) natural and 2) managed vegetation growth, 3) silicate weathering, and 4) within the soil, can all be predicted within the same framework, and without use of adjustable parameters6. Simultaneously, long-standing puzzles of how to predict non-Gausssian solute transport, and to determine when reactions in porous media are transport-limited, are solved.

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Upscaling non-linear chemical reactions in porous media

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ABSTRACT

The law of mass action for non-linear reactions assumes perfect mixing within some volume, or more precisely, that each molecule or macroparticle has equal probability of collision with all others. When some collision probabilities become small compared to the thermodynamic reaction probability, the system experiences the general feature called imperfect mixing, and the law of mass action is not generally applicable. Large-scale simulations of flow, transport, and reaction typically start with very coarse Eulerian grids (for velocities), and apply the law of mass action at that scale, with some empirical adjustments of the thermodynamic rates. In this talk, we review some progress on direct calculation of the effect of poor mixing on spatially averaged reaction rates and how this might impact the upscaling of reaction rates and/or effective equations and solution techniques at the large scale.

Reduced-order Transport Models for Energy and the Environment

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ABSTRACT

In this talk, I will discuss several reduced-order transport modeling studies motivated by energy and environmental processes: (i) Inspired by CO2 geological storage, we study fluid (CO2) injection into a confined porous reservoir initially saturated with another fluid (brine), and characterize the time evolution of the fluid-fluid (CO2-brine) interface. Because of the effect of confinement, we identify a transition from an early time self-similar solution to three branches of late time self-similar solutions for the interface shape. (ii) Inspired by shale gas recovery, we study the fluid-driven cracks in an elastic matrix and characterize the evolution of the crack shape; we also study the elasticity-driven backflow process following fluid injection, and obtain a simple scaling law for the backflow rate of the fracking fluids. (iii) I will also introduce our fundamental study on the viscous fingering instability, which is related to enhanced oil recovery, and report a series of time-dependent strategies for the stabilization of the viscous fingering instability at fluid-fluid (e.g., water-oil, gas-oil) interfaces.

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Mixing through Viscous and Gravitational Flow Instabilities in Compositional Multiphase Flow

Presenter: Joachim Moortgat
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ABSTRACT

Viscous and gravitational fingering refer to flow instabilities in porous media that are triggered by adverse mobility or density ratios, respectively. These instabilities have been studied extensively in the past, but predominantly for 1) single-phase flow (e.g., contaminant transport in groundwater, first-contact-miscible displacement of oil by gas in hydrocarbon production), and 2) multi-phase immiscible and incompressible flow (e.g., water-alternating-gas, or WAG, injection in oil reservoirs). Fingering-type mixing in multiphase compositional and compressible flow has received much less attention, perhaps due to its high computational complexity. However, many important subsurface processes involve multiple phases that exchange species. Examples are carbon sequestration in saline aquifers and enhanced oil recovery (EOR) by gas or WAG injection below the minimum miscibility pressure. In multiphase flow, relative permeabilities affect the mobility contrast for a given viscosity ratio. Phase behavior can also change local fluid properties, which can either enhance or mitigate viscous and gravitational instabilities. This work presents a detailed study of fingering behavior in compositional multiphase flow in two and three dimensions and considers the effects of 1) geostatistical multi-facies heterogeneity in which channeling competes with fingering, 2) Fickian diffusion, 3) mechanical dispersion, 4) flow rates, 5) domain size, geometry, and dimensionality, 6) gravity competing with viscous instabilities, and 7) composition dependent phase mobilities. Simulations are performed on fine grids with a higher-order finite element reservoir simulator to resolve the small-scale onset of instabilities. All fluid phase properties are derived from rigorous equation-of-state based phase stability and phase-split computations. Results suggest that fingering in compositional multiphase flow can be profoundly different from miscible conditions.

A copula-based analysis of the dependence structure and process memory of anomalous pore-scale transport

Presenter: Sebastian Most
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ABSTRACT

Many applied simulations of transport processes in porous media are working on the regional scale. Highly-resolved pore-scale transport simulations exist, but computational limitations constrain the volumetric size of the investigated porous media to a few cubic centimeters. This is why upscaling becomes necessary. Upscaling often means to average over a predefined (representative elementary) volume. Within this volume, all the small scale heterogeneities are averaged out, but then considered through upscaled governing equations that include dispersion concepts. Classical Fickian transport models are advection-dispersion equation (ADE) and particle tracking random walks (PTRW). Within the PTRW framework, transport is represented as an advection-driven drift term plus a stochastic process (with Gaussian, independent increments) for diffusion/dispersion that scales with the square root of time.

The problem is that small-scale heterogeneities like preferential flow paths or stagnant zones lead to early- and late time tailings of contamination breakthrough curves, respectively. Transport processes subject to such phenomena are called non-Fickian transport, and cannot be represented by Gaussian stochastic processes in PTRW. Frequently applied non-Fickian approaches are continuous time random walks (CTRW). While CTRWs are able to reproduce early arrival and tailing, most CTRWs assume statistical independence between consecutive time steps. Transport along preferential flow paths, however, cannot be considered to be independent, because the physical flow laws inside the pore geometry enforce a spatial structure of pore-scale velocities – and hence dependence and memory of velocity and corresponding advective particle increments. To account for these dependencies, correlated CTRWs (cCTRW) have been established. Up to presence, they represent the advective particle increments as a Markov process of order one. This means that the current advective increments depend on the previous increments, but memory over longer time lags is excluded.

We argue that, for appropriate simulation of transport processes at the pore scale, dependence and memory effects must be described in their full complexity. The strong heterogeneity of porous media induces a highly complex dependence structure and we want to present techniques to reveal and analyze that dependence. In the presented study, we extract this dependence by applying a copula-based analysis method to advective-diffusive particle trajectories computed at a very fine resolution within a pore geometry obtained through micro-tomography. We investigate the dependence as function of (a) the temporal increments on which the particle trajectories are sampled, and (b) of the time lag over which the process memory vanishes. A key novelty is that we evaluate dependence and memory not for the longitudinal direction of particle displacements, but also between the longitudinal and transverse components of particle displacements. In specific, we suggest to perform such analyses in a spherical coordinate system which we found to be more appropriate in representing cross-directional dependence and memory effects. We repeat this analysis under several transport regimes characterized by different Peclet numbers.

Bringing chaos to enhance heat extraction from geothermal reservoirs

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ABSTRACT

Traditional methods for heat recovery from underground geothermal reservoirs employ a static pair of injector-producer wells. Such a system may not be effective in harnessing the full potential of the geothermal reservoir due to preferential flow of the production fluid via larger fractures and regions of higher permeability. Recent studies in literature [1,2] have shown that using a well-devised pumping scheme, that by design incorporates concepts from chaos theory, can dramatically enhance production rates. This approach exploits the fact that chaotic advection can significantly boost performance by distributing production fluids throughout the entire reservoir and promoting heat transfer by inducing large gradients [3]. However, the studies in [1,2] concern isotropic conditions, while realistic reservoirs are anisotropic. This motivates our study, which expands on [1,2] by investigating the effect of anisotropy on Lagrangian transport characteristics.

The flow field generated in a traditional geothermal reservoir with a pair of injector-producer wells can be modeled by a potential flow in a 2D circular domain driven by a source-sink pair located diametrically opposite to each other on the domain circumference. By periodically reorienting the source-sink pair the so-called rotated potential mixing (RPM) flow becomes capable of accomplishing chaotic advection [1,2]. 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 (Fig. 1a). The effect of reorientation of source-sink pair can then be achieved by periodically turning off the current pair and turning on the pair located theta apart.

Our study investigates the effect of anisotropy in 2D RPM flow by numerical simulations. The numerical analysis centers on a dynamical-systems approach making use of Poincaré sections to visualize the transport of production fluid. 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 transport characteristics and the role of anisotropy.

Preliminary results indicate that anisotropy has significant impact on transport characteristics in RPM flows. Employing an 8-well configuration, corresponding to a reorientation angle of 3pi/4, in isotropic media produces a symmetric Poincaré section (Fig. 1b) with visible island structures. Such islands define transport barriers, thereby limiting mixing and scalar transport. For the same 8-well configuration, introducing anisotropy changes the picture drastically, with the placement of the wells relative to the permeability direction playing a critical role. Alignment of the wells with the permeability direction can have a detrimental effect on the distribution of the production fluid and thereby on the heat extraction rate (Fig. 2b), by its prolonged confinement to a subregion of the

reservoir (dark band). Non-alignment of the wells with the permeability direction can avoid such confinement and may thus promote efficient distribution of the production fluid by chaotic advection (Fig. 3). This makes clear that reservoir anisotropy is a crucial factor in the design of an optimal well placement and pumping strategy.

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Irreversibility of transport and the role of porescale flow heterogeneity and mass transfer processes

Presenter: Juan J. Hidalgo
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ABSTRACT

We consider pore scale transport in a composite medium consisting of two component of identical hydraulic conductivity by different porosity. It has been observed (Berkowitz et al., 2009) that breakthrough curves measured at the low and high porosity ends behave differently while the Darcy-scale advection-dispersion equation predicts otherwise. We study the origin of this asymmetry using pore scale simulations considering different regular and random packings of grains, and size distributions. We explore different velocity distributions generated by the pore structures and specifically the role of low velocity, or stagnant zones as a function of porosity. Second, we analyze the impact of the velocity field properties on solute transport to establish a relation between the grain distribution and porosity, the velocity PDF and the breakthrough behavior in order to determine the mechanisms that lead to transport irreversibility.

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The LATERS Markov Model for Bimolecular Reactive Transport

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ABSTRACT

Upscaled modeling of bimolecular reactive transport is a two step process which consists of first modeling mixing (which is a pore-scale process) properly and then upscaling its effect on reactions appropriately. 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.
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 [2], to transport particles, then maps their positions to an Eulerian grid to simulate reactions using the volume averaged reaction term in [1]. 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 the Eulerian reaction method is efficient, because it does not require calculation of distances between particles.
The overall goals of this work are to develop an efficient model for bimolecular reactive transport at large scales and to test its accuracy in a simple 2D system, with hopes that it may be used as a predictive tool for reactive transport modeling in more complicated flow fields. 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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Mixing and deformation in non-ideal reactive transport systems

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ABSTRACT

Reaction rates in porous media flows are often limited by either 1) the surface area available for reactions to occur across, or 2) the rate at which solutes collocate, and react, and understanding mixing phenomena is central to accurate prediction of mass formation. Thus, there is a competition between mixing and deformation that can lead to enhanced or inhibited reaction rates, depending on local conditions. Scalar dissipation rates have been shown to be good proxies for the mixing rate of solutes and form the basis for a wide range of reactive transport modeling techniques. The central assumption behind this approach to reactive transport is that the mixing rate between two reactive solutes can be approximated from an equivalent passive tracer or a conservative component. Solutes in natural systems are constantly affected by heterogeneities in the velocity field and idealized initial or boundary conditions are unlikely. Given their important role for predicting reaction rates, a prudent question is what should scalar dissipation rates look like for non-ideal conditions? The second aspect of mixing limited reaction systems is the length of the mixing interface and, unlike dissipation rates, this can increase and decrease over time, which may compliment or inhibit the temporal variations of mixing rates. This presentation investigates the tradeoffs between mixing and deformation and some of the effects of reactions, sources, boundary conditions on mixing rates [Engdahl et al., 2013]. The analysis begins with a series of analytical models of reactive transport in simple systems where we predict the mixing rates and provide experimental validation. We then examine the changes in deformation for the same simple flows before considering the combined effects of mixing and deformation. The significance of this work is that it provides a picture of detailed mixing and deformation interactions that give some guidance for a framework that can be used to “correct” scalar dissipation rates in non-conservative systems. These corrections can then be used to make improved estimates of upscaled reaction rates for equilibrium, kinetic, reversible, and irreversible systems when non-idealities or deformations are expected in the tracers used to infer mixing.

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Upscaling multi-component reactive transport in aquifers with connected subsurface structures

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ABSTRACT

In field applications chemical reactions are consistently overestimated. The reason is that averaged concentration gradients and means mass fluxes are used. And generally complete mixing is assumed. But in reality we have incomplete mixing. The controlling factor seems to be connectivity. Our hypothesis is that a sound definition of connectivity is key to upscaling complex reactive systems.
Our objective is twofold. First, we investigate the effect of different types of connected structures and connected hydraulic conductivity fields on multi-component reactive transport. And second, we test different upscaling approaches. We study explicit multi-component transport in heterogeneous aquifers for the example of calcite-dissolution. We compare different types of heterogeneity from intermediately well connected (multigaussian) fields to very well connected fields. The fundamental difference of these fields stems from their connectivity structure. We apply some previously developed analysis of the connectivity structure, the connectivity metrics. And establish some general rules for upscaling reactive multi-component transport in presence of connected aquifer structures.

Segregation in reactive systems with shear flow

Presenter: Diogo Bolster
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ABSTRACT

Incomplete mixing of reactive solutes is well known to slow down reaction rates relative to what would be expected from assuming perfect mixing. In purely diffusive systems, for example, it is known that small initial fluctuations in reactant concentrations can lead to reactant segregation, which in the long run can reduce global reaction rates due to poor mixing. In contrast, nonuniform flows can enhance mixing between interacting solutes. Thus, a natural question arises: Can nonuniform flows sufficiently enhance mixing to restrain incomplete mixing effects and, if so, under what conditions? We address this question by considering a specific and simple case, namely, a laminar pure shear reactive flow. Two solution approaches are developed: a Lagrangian random walk
method and a semianalytical solution. The results consistently highlight that if shear effects in the system are not sufficiently strong, incomplete mixing effects initially similar to purely diffusive systems will occur, slowing down the overall reaction rate. Then, at some later time, dependent on the strength of the shear, the system will return to behaving as if it were well mixed, but represented by a reduced effective reaction rate.

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Incomplete mixing and reactions in laminar shear flow
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Point Mixing Rate Potential in Heterogeneous Velocity Fields

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ABSTRACT

Groundwater flows take place in aquifers which often exhibit multiscale heterogeneity. We seek to identify the key properties of the underlying velocity field that dictate the mixing state of a solute plume in highly heterogeneous flow fields in order to accurately predict mixing. We propose a measure based on the trace of the strain field squared, as sampled by the plume, as a predictor of pre-asymptotic mixing, as quantified by the solute plume's dilution index.

Carbonate dissolution probed with nuclear magnetic resonance imaging and spectroscopy: changes in reaction mode with reactant flow rate

Presenter: Andy Sederman
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ABSTRACT

Much of the world's oil and a sizable portion of UK water is extracted from porous sedimentary rock. Currently, the storage of super-critical CO2 in these underground reservoirs after their exploitation is being explored. Chemical reaction within the rock matrix, be it reservoir stimulation through acidisation, the introduction of a contaminant, or the interaction of super-critical CO2 in brine with the rock, is of primary importance in these processes. Here we combine under-sampled nuclear magnetic resonance (NMR) flow measurements [1] with interpolation, MRI [2] and NMR relaxation measurements to probe the pore-space and hydrodynamics during core-plug dissolution. Quantitative 1D, as well as qualitative 2 and 3D images of the water saturated rock core plugs are employed to observe the extent of rock saturation, pore widening and the development of "wormholes". Flow NMR allows the production of displacement distributions, yielding information on the effect of the pore space changes on the fluid flow. The dependence of reaction mode on the flow rate of the reactant for the dissolution of the carbonate Ketton with 0.01 M HCl was explored.

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Dynamic simulation of diffusion controlled celestite precipitation in pore scale porous media

Presenter: Frieder Enzmann
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ABSTRACT

Reactive transport processes are complex in nature and a challenge for both experimental and modelling approaches. Ongoing advancements in experimental and computer technologies enable dynamic simulations at the pore scale. In this study a workflow was developed, improved, and compared on a well characterized mineral precipitation experiment.
In the experimental setup, both ends of a compacted sand column were connected to a reservoir containing SrCl2 and Na2SO4 solutions, respectively, at equal concentrations. Celestite (SrSO4) was precipitated in the mid of the sand column under diffusion-controlled conditions. Computed micro-tomography (?CT) imaging was used before and after the precipitation reaction to quantify the thus changed pore space and fluid transport.
Our general workflow combines a robust solver for particle transport, a geochemical calculator, and data conversion scripts. The coupled GeoDict software code (Math2Market GmbH) iteratively simulates particle diffusion paths employing its AddiDict module. The virtual particles in AddiDict are coupled at high spatial and temporal resolution with the chemistry of the solid matrix and fluid compositions. The geochemical equilibrium code PHREEQC (USGS, v3) is implemented to indicate the probability of pore cement precipitation wherever it can be expected. MATLAB (MathWorks, v2013a) scripts automatically access GeoDict control files and data files. Finally Python (Python Software Foundation, v2.6.6) embeds both above mentioned codes into a time loop and thus realizes the sequential simulation of pore-scale reaction and transport.
Simulation results will be presented and illustrate the capabilities of the presented model considering shape and thickness of the precipitation front as well as the continuously changing effects on hydromechanical transport parameters.

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3D Observations of Reactive Transport in Natural Consolidated Rocks

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ABSTRACT

Rock structure heterogeneity can have a significant effect on dispersion, mixing and reaction of aqueous components in porous media. To observe the effect of pore structure heterogeneity on reactive transport, core flooding experiments were carried out for a sandstone and two carbonate rocks of different heterogeneity for eight different Peclet numbers ranging from 0.5 to 100. The rock cores were 20cm long and had a diameter of 7.62cm. A device consisting of three annular regions was used for injection (fig.1). Water was injected into the center and outer region and a chemical tracer into the middle region. A non-reactive tracer was used for the transport experiments. For the reactive experiments an acidic tracer was used resulting in mineral dissolution. The steady state transverse dispersal of the tracer was visualized in three dimensions with an X-ray medical CT-scanner (fig.2). For the reactive transport experiments, an ICP-MS was used to measure the effluent. Local transverse dispersion coefficients (Dt) were calculated from the change in variance of the transverse distance traveled by the tracer along the core. The change in variance along the core followed a characteristic pattern for each flow regime in each of the rocks. Core averaged transverse dispersion coefficients were calculated and showed an increase with pore structure heterogeneity. Furthermore, concentration maps were used to visualize and quantify larger scale flow structures e.g. meandering, flow focusing, flow splitting by using observations at different Peclet numbers (fig.3). The flow fields within the rocks were visualized by mapping the location of the peak of the plume. A characteristic flow field for each flow regime in each of the rocks was observed. Tortuosity measured from the peak locations showed an increase with pore structure heterogeneity and a decrease with Peclet number. The core flooding experiments were modeled using the CrunchFlow reactive transport code. High quality data sets of the space and time evolution of the concentration in core-flooding experiments like these can be used as future benchmark test for numerical models for transport in natural rocks.

Impact of Heterogeneity and Connectivity on Density-Driven Flow Following CO2 Storage in Saline Aquifers

Presenter: Mohamad Reza Soltanian
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ABSTRACT

It is well known that, when CO2 is injected in saline aquifers, mass transfer between CO2 and brine can cause a local increase in the aqueous phase density, which may be gravitationally unstable. Depending on the density contrast, formation permeability, brine viscosity, and Fickian diffusion coefficients (diffusion being a restoring force), density driven flow may mix dissolved CO2 throughout the aquifer at relatively fast convective time-scales. As such, gravitational fingering can increase the storage capacity of a given aquifer and reduce the risk of leakage in case of failure of the cap rock. Heterogeneity has a strong impact on density-driven flow. If the formation is layered and the effective vertical permeability is low, fingering is suppressed. In more complex permeability fields, e.g., consisting of several disparate facies, finger propagation is slow or absent through low permeability facies, but may be enhanced by channeling through higher permeability pathways (see Figure 1). In this work, we perform higher-order finite element simulations on fine grids of dissolution–diffusion–convection transport of CO2 in saline aquifers with a focus on realistic representations of multi-facies heterogeneity. Heterogeneity fields often have sharp, discontinuous contrasts ranging by orders of magnitudes (e.g., across sandstone-shale contacts). We construct realistic permeability fields by a Markov Chain approach, which represents facies architecture using commonly observed characteristics of facies (e.g., volumetric proportions and mean lengths). Initial results show that facies structure, specifically the positioning of high permeability facies and their connectivity control the dynamics of gravitational instability at the field scale. These results will lead to a better understanding of how heterogeneity and structure of highly permeable facies influence gravitational instability and dissolution rate of CO2 in brine.

Towards A Fully Compositional Mixing Model: Viscous Flow Instabilities in Different Levels of Miscibility and Fluid-Rock Heterogeneities

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ABSTRACT

Fluid mixing and its interplay with flow instabilities and/or channeling through heterogeneous media have been studied in some detail for mostly fully miscible conditions in which a single phase is generally represented by two components, e.g. a solvent and a solute. In such studies, fluid properties are assumed to be either constant or to follow simple mixing rules depending only on concentration. Viscous fingering, a hydrodynamic instability due to the displacement of a more viscous fluid with a less viscous one, has been studied predominantly for immiscible or fully miscible fluids.

However, many problems of interest, such as gas injection in hydrocarbon reservoirs, involve multiple species and fluid properties, even in single-phase, and depend non-linearly on temperature, pressure, and composition through an equation of state (EOS). Moreover, depending on the minimum miscibility pressure, solubility factor, and in-situ conditions, a two-phase region may develop, e.g. in a partially (multi-contact) miscible system. Fingering in this regime has been recently characterized using a miscible Korteweg stress, which simply modifies (lowers) the interfacial tension (IFT) of an immiscible system as a coefficient to account for suppressed growths of fingers.

This work aims at studying species mixing in various regimes of miscibility, with fluid properties determined by rigorous EOS-based (Peng-Robinson and CPA) phase-stability and phase-split computations. Fickian diffusion, driven by chemical potential gradients, is modeled to capture the diffusive fluxes across sharp phase boundaries e.g. across a finger perimeter in absence of perfect miscibility. Furthermore, we allow for composition-dependent dynamic IFT through a mechanistic Parachor model to better represent the compositional effects on miscibility, IFT, and capillarity in a multicomponent fluid-fluid system. Flow and transport are modeled on very fine grids with our in-house, higher-order, finite element reservoir simulator.

In addition to compositional effects across different degrees of miscibility, we investigate the impact of correlated heterogeneities for a wide range of (geostatistically generated) correlation lengths and lognormal permeability distributions.

Our numerical framework is capable of resolving small-scale fingering patterns on one hand, and the potentially dispersive flow caused by heterogeneity and inherent channeling on the other hand. Our results provide a broad perspective into mixing mechanisms coupled with complex fingering patterns in porous media.

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Mineral precipitation in a fracture

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ABSTRACT

Geochemical interactions during the withdrawal/injection of fluids into the subsurface can modify fracture apertures through dissolution and/or precipitation of minerals. Modification of fracture apertures during reactive flow is strongly affected by non-reactive, non-wetting fluids that limit the fracture surface area and void volume that can be affected by reactive phases. We present results on the effect of a non-reactive, non-wetting phase during reactive flow on the distribution of precipitates and affect on acoustic wave propagation.
The spatial distribution of precipitates is influenced by: (1) the flow path geometry which controls the mixing of the two fluids; (2) the presence of gas which blocks or which causes precipitates to occur along the solid-fluid interface (fracture wall/liquid interface), reduces the pore-size available for precipitation and affects the thickness and location of the precipitates; and (3) location of precipitates, whether the precipitates are pore-filling and settle out of solution versus surface adhering. The type of precipitation affected particle size, deposit thickness and the acoustic response?
For pore-filling precipitates, the particles were more uniform in size, and there were thicker deposits. They affected the density of the pore filling material so increased the acoustic velocity.
For surface adhering precipitates, the presence of gas limited accessible void volume, and the deposits were thinner with variable particle sizes. They increased the stiffness of the fracture so increased the acoustic amplitude.

An evaluation on the effective stress principle of saturated porous media by molecular dynamics techniques

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ABSTRACT

Effective stress principle is the fundamental theorem in porous mechanics. It is of philosophic importance to confirm the validity of this principle due to its wide application in describing building materials behavior. To date, there still exists some different mathematical expressions for this fundamental theorem, which causes unresolved debate on which expression is correct and the applicability of each expression. The emerging of atomistic modeling techniques makes it possible for us to observe the complicated material behaviors with an extremely high resolution and interpret the complex physical process underlying these behaviors. In this paper, molecular dynamics simulation is employed to explore the stress distribution in porous media and the validity of these existing expressions for the effective stress principle. In terms of the building materials, the soils media is usually conceptualized as pore water infiltrating the packing spherical soil particles while the rock and concrete is usually conceptualized as solid media with circular pores. Such conceptual models have been widely adopted to derive or interpret the general physical models depicting these building materials behavior. Herein, the initial solid-water simulation system is modeled to mimic these conceptual models. The solid is modeled as a Face-Centered Cubic (FCC) crystal while the water is modeled by a monoatomic water model. A coarse grained model is adopted to describe the interatomic potential between solid and water. A series of molecular dynamics simulations is conducted to clarify the influence of some parameters such as strain level, compressibility of solid and porosity. At last, an evaluation on the validity and applicability of these existing expressions of effective stress principle is presented.

Effects of hydrologic processes on mineral dissolution rates

Presenter: Heewon Jung
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ABSTRACT

Hydrologic processes play an important role in controlling chemical reactions rates in natural systems. Rates of fluid and solute transport control the rate of supply and removal of reactants and products to and from reacting sites, which determines chemical saturation state of the given system. Thus, rates of fluid transport influence whether reaction rates are transport-controlled (increased fluid velocity leads to increased reaction rate) or surface-controlled (rates not dependent upon fluid velocity) and fluid mixing in heterogeneous systems can result in complicated relationships between local, small-scale and effective, large-scale geochemical behavior. Heterogeneity in fluid transport also impacts the total mineral surface area exposed to reactive fluids. Where fluid flow is dominantly through preferential flow paths, the effective mineral surface area is lower than the total mineral surface area. These hydrologic factors, often eliminated in laboratory dissolution rate experiments, likely contribute to observed variation between field-determined and laboratory-measured geochemical reaction rates. Here, we systematically explore the relationships between rates of fluid flow and geochemical reactions in heterogeneous porous media with fully coupled reactive transport models. Hydrologic heterogeneity is systematically varied from isotropic, homogeneous to anisotropic, layered permeability fields in multiple statistically identical realizations and reactive conditions are induced for two different minerals with different far from equilibrium reaction rates (calcite, anorthite). Preliminary results showed about 10 orders of magnitude difference in anorthite dissolution reaction rates over the domains in given conditions solely because of the heterogeneous distribution of the fluid flow velocity. In general, higher velocity is correlated with higher reaction rates but it gets complicated by the mixing effects. This type of approach will help elucidate hydrologic controls on effective reaction rates at field scales and improve the application of laboratory measured rates to numerical simulations of field scale systems.

The role of medium heterogeneity and viscosity contrast on fluid mixing in miscible displacement

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ABSTRACT

Over the last four decades, with the increasing demand for energy and fast depletion of conventional oil resources, heavy oil and bitumen reserves have gained considerable attention. Recovering these reserves efficiently, environmentally, and economically however remains a crucial challenge due to their high viscosities. Injection of a solvent into the reservoir that can lower the oil viscosity through dilution is an alternate to the current thermal-based recovery techniques. Oil recovery from solvent-based EOR processes is a function of solvent and oil mixing degree; hence, making mixing an important feature of a miscible displacement. Fluid mixings in the miscible displacement of two solutions in porous media, quantified by mixing length, can be promoted by both adverse viscosity ratio and medium heterogeneity. During miscible displacement when there is an unfavorable viscosity ratio, i.e. displacing fluid is less viscous that displaced fluid, hydrodynamic instabilities develop at the interface of fluids. The instability manifests itself in the form of advancing fingers of displacing solution causing poor displacement efficiencies. However, it can accelerate mixing among solutions. On the other hand, the macroscopic transport attributes of a porous medium is significantly affected by its pore volume microstructure (pores and throats). In Fact, the non-uniform distribution of shape and size of pores and throats in a porous medium, i.e. medium heterogeneity, results in preferred pathways for flow and gives rise to channeling of flow.

We conduct miscible displacement simulations in heterogeneous porous media to quantify which one of viscous fingering or medium heterogeneity induced channeling is dominant in increasing the growth rate of mixing zone. We construct two dimensional unconsolidated granular porous media with different levels of microscale heterogeneity. We solve mass conservation equations for the transport of solute and solutions along with the continuity and momentum equations in the form of Stocks equation. The results show that mobility ratio and heterogeneity have significantly different effects on mixing at different time scales and flow velocities. We report that dispersive flow is dominant at lower velocities and as flow velocity increases, channeling due to micro scale medium heterogeneity occurs, resulting in higher growth rates for mixing length. At high velocities, viscous fingering driven mixing becomes the dominant regime essentially for high mobility ratios. Various flow patterns and mixing length growth rates are analyzed and quantified for different parameter combinations.

Challenges in reactive transport modeling - The limits of a 1D continuum approach

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ABSTRACT

Reactive transport models are complex and present many challenges. They must include numerous parameters that are often difficult to obtain experimentally. This study focused on modeling the reduction of porosity from salt precipitation (celestite and calcite) in small columns of compacted sand (10 mm diameter, 50 mm length), and its effects on ions diffusion. The main aim was to determine whether or not the Archie's law, describing in a simplistic fashion the relationship between porosity and diffusivity, was applicable to reactive transport.
In order to constrain the model, a great number of experimental data were obtained from through diffusion of HTO before and during porosity reduction, µ-CT of initial and clogged sand columns and post-mortem analysis. However, the reactive transport model built upon the experimental results largely underestimated the remaining connected porosity in the precipitation zone and overestimated the amount of precipitate. The results presented demonstrate that 1D continuum models might fail in the long-term prediction of transport in geochemically disturbed systems and argue for more complex 2D pore-scale reactive transport and/or a modified diffusivity/porosity relationship (Chagneau et al., 2015).

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Numerical Simulation of Foam Flooding in Porous Media in Absence and Presence of Oleic Phase

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ABSTRACT

This paper reports a series of numerical simulations of foam coreflood experiments in absence and presence of oil. The experiments consisted in co-injection of gas and Alpha-Olefin Sulfonate (AOS) surfactant solution into a Bentheimer sandstone samples initially saturated with the surfactant solution. The in-house numerical simulator of IFPEN (PumaFlow) was used. The foam model implemented in the simulator is based on a local equilibrium and described dependency of foam mobility reduction factor using several independent functions of the relevant physical variables (liquid saturation, foam velocity, etc.).
Firstly numerical simulations investigated the effect of surfactant concentration on pressure drop across the core in the foam flooding in the absence of oil. To this end, the dry-out and gas velocity functions in the foam model were determined from the experimental data obtained at low and high quality regimes, at constant total velocity. Then, pressure drops of foam flooding at two different surfactant concentrations were modeled by determining the parameters of surfactant dependent function of foam model. The simulation results fit the experimental data of pressure drops very well.
Secondly numerical simulations investigated oil displacement by foam where the main goal was determining the foam model parameters and oil relative permeabilities as a function of oil saturation. Theferore, pressure drop across the core, oil cut and oil recovery factor were modeled. An excellent match was obtained between the pressure profile and oil recovery obtained numerically with those obtained from the coreflood experiments. This confirmed that the PumaFlow foam model is robust and reproduces the essential features of foam flow in porous media in absence or in presence of oil.

Experimental investigation of ganglia transport in porous media

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ABSTRACT

Recent experimental two-phase flow studies have shown that there is a difference between the capillary pressure, saturation, and specific interfacial area (Pc-Sw-awn) surfaces obtained under quasi-static and transient conditions. This mismatch happens mostly due to the disconnection of phases during such experiments. The aim of this work is to investigate the liquid blobs formation due to disconnection and their mobilization during multiphase flow experiments.
In this work, silicon-glass micro-models [2] and a high-resolution visualization setup was used [1, 3]. The micro-models had a flow network based on Delaunay triangulation. The overall dimensions of the flow network were 35mm x 5mm, with a mean pore size of 50 microns and a depth of 25 microns. The pore network was etched on silicon wafers with the use of Deep Reactive Ion Etching (DRIE) technique and they were sealed with borosilicate glass (Pyrex). The micro-models were treated so as to create a uniform silicon oxide layer on the etched surface, to ensure uniform hydrophilicity.
The two-phase flow experiments were conducted by simultaneous injection of both wetting and non-wetting phase into the flow network. Prior to the injection, the micro-model was initially saturated with the wetting phase. The continuous phase (wetting phase) flow was controlled by a pre-selected pressure gradient, while the disconnected phase was injected at controlled volumes with a syringe pump. The images acquired by the visualization setup were processed in order to obtain information on the movement of the non-wetting phase ganglia and the fluid-fluid interfaces, as well as the evolution of fluid-solid interfaces. Phase saturation and local capillary pressure were also calculated.
The aim of this research is to develop a theory that will successfully describe the physics behind the formation and flow of blobs and discontinuous phases in porous media. Successful incorporation of the effect of the disconnection of phases in the equations that are used to model two-phase flow will potentially contribute to the development of a new theory which includes specific interfacial area as a separate state variable.

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Cyclic gas injection in fractured shale micromodels at reservoir conditions

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ABSTRACT

We describe a unique microfluidic experimental system for real-time observations of pore-scale fluid flow and transport in geo-material micromodels (e.g., shale, Portland cement, limestone) at pressures (up to 10.34 MPa) and temperatures (up to 80 °C) commonly encountered in subsurface reservoirs. The use of geo-material micromodels allows us to investigate fluid-rock interactions including wettability, chemical reactivity, and nano-scale porosity at conditions representative of natural subsurface environments that cannot be recreated in engineered micromodels. In this work, we present cyclic gas injection experiments that are designed to mobilize hydrocarbons (e.g., n-Decane) within shale fracture networks. The experiments consist of pressurizing the porous system with gas, soaking the system at a predetermined operating pressure for a specified period of time, and then rapidly depressurize the system. We conducted a series of experiments using CO2 and N2 as the injected gas. In both cases the gas compress during the depressurization stage and then decompress during the depressurization stage, leading to oil mobilization. However, CO2 is partially miscible with n-Decane and undergoes a phase change to supercritical CO2 at approximately 7.4 MPa and 31 °C, whereas N2 is largely immiscible with n-Decane and does not change phases for the pressures and temperatures considered in this work. We use fluorescent microscopy to image the phase behavior (e.g. diffusion of CO2 into n-Decane) within the fracture networks and quantify the amount of oil mobilized during each cycle. In addition, we identify previously unrecognized mechanisms that lead to increased oil mobilization and highlight observations of unexpected flow blocking events.

Pore-scale Wettability Evolution model during Primary Drainage

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ABSTRACT

Carbonate reservoirs are widely recognised to be weakly- to moderately oil-wet at the core-scale, although pore-scale wettability distributions remain poorly understood. Particularly, the wetting state of micropores is crucial for assessing multi-phase flow processes associated with oil recovery techniques, as microporosity prevails in many carbonates and often determines the overall connectivity of the pore space. Oil has been detected within micropores in carbonate rocks, making oil-wet conditions plausible, but it is not clear how oil may have invaded these pores without invoking excessively high capillary pressures. Traditionally, pore-scale modelling of wettability has been based on the surface adsorption of polar molecules from the crude oil phase, commonly identified as asphaltenes. However, such large molecules are hydrophobic, therefore unable to penetrate water wetting films on the pore surfaces. Additionally, the size of these molecules may prevent invasion into the micropores. On the other hand, smaller polar non-hydrocarbon compounds present in crude oil (e.g. alkylphenols) are known to be hydrophilic and highly surface-active.
In this work, we develop a novel wettability alteration model evolving during primary drainage, which involves release of these small polar species into the water phase. We implement a diffusion and adsorption model for polar compounds that triggers a mild wettability alteration from initially water-wet to more neutral–wet conditions. This dynamic mechanism is incorporated in a two-phase flow pore-network model to which we add a notional time-dependency of the quasi-static invasion percolation mechanism. Interestingly, we manage to invoke clear differences in the primary drainage patterns by varying the balance between the processes of oil invasion and wetting change. Indeed, this balance dictates the initial water saturation for waterflooding. Under conditions where oil invasion is slow compared to a fast and relatively strong wetting change, the model results in significant non-zero water saturations, even at high capillary pressures. This water trapping results from the removal of water wetting films in the corners of angular pores. On the other hand, for relatively fast oil invasion or weak wetting changes, the model allows higher oil saturations at fixed maximum capillary pressures, and possible invasion of micropores at moderate capillary pressures. The implemented wettability alteration model results in profoundly different residual oil saturations following waterflooding.

Study of surfactant transport through natural rock in water and water/oil system

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ABSTRACT

Surfactants in water are used in enhanced oil recovery (EOR) to significantly increase the oil production of mature reservoirs. The injection of surfactants is classically performed in tertiary recovery after the water flooding. The residual oil saturation after water flooding can be relatively high, of the order of 40-50% in the case of water wet rocks. This residual oil is no longer mobile and is distributed within the rock structure as discontinuous oil fragments trapped in pores by capillary forces [1]. The objective of the surfactant injection is to decrease significantly the interfacial tension between oil and water. So, transport of surfactant within the porous media is a crucial point because it controls the way surfactants contact the oil water interfaces. The objective of this work is to study the different mechanisms that control the transport of surfactant at the Darcy scale: advection, dispersion and adsorption in water or water/oil system.

In the first part of this work, we study experimentally the injection of sodium dodecyl benzene sulfonate (an anionic surfactant) in water-saturated and oil/water-saturated sandstone samples (Clashach). Concentration of the surfactant at the outlet is measured with spectrophotometry. Passive tracer (potassium iodide) tests have also been performed to measure the sample dispersivity with spectrophotometry. In a second part, the tracer transport is modeled using the advection-dispersion equation with an equilibrium or kinetic Langmuir model for the adsorption term [2].

The experimental results show that passive tracer tests and surfactant tracer tests are relatively different. Surfactant concentration as a function of the time scaled with the time to inject one pore volume, is flow rate dependent and presents a shift as compared to passive tracer tests. The experiments show a difference between adsorption and desorption of the surfactant (surfactant injection after brine and brine injection after surfactant). We show that kinetic Langmuir model is more relevant for modeling the transport of surfactant. By identification with the model, we were able to measure the dispersivity of the surfactant and to evaluate the coefficients of the adsorption model.

Experiments have also been done with samples prepared at residual oil saturation. Samples made from the same sandstone are fully saturated with water, then drained by dodecane in a centrifuge and saturated again with water by spontaneous imbibition. Tracer tests are done to characterize the dispersivity in water in presence of oil and surfactant breakthrough curves are measured at flow rates such that the capillary number is always lower that the threshold of oil mobilization, so oil saturation remain constant during all the tests.

The understanding of surfactant transport in porous media is key for chemical enhanced oil recovery processes. Through the use of numerical models and laboratory experiments, we were able to evaluate and quantify the main mechanisms for surfactant transport at the Darcy scale.

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Dynamic Simulation of Multiphase Flow and Ganglion Mobilisation in Digital Porous Media

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ABSTRACT

In this work, we describe a new fully dynamic pore network model that has been developed to investigate unsteady-state flow and ganglion mobilisation in mixed-wet systems, where viscous forces are no longer negligible compared to capillary forces. We introduce a novel formulation, where fluid fractions are updated in capillary elements according to the relative balance between capillary and viscous forces without the need for expensive trapping rules. The model is completely general and can consider multiple phases flowing under various injection protocols. We show that such an approach is able to reproduce a wide range of experimental observations, including ganglion mobilisation, counter-current flow and film transport. The model is easily adapted for any network model architecture and results are presented from off-lattice, rock-derived networks.
We have investigated the impact of several parameters – network properties, wettability and injection rate – on numerous secondary and EOR recovery processes and two examples will be discussed in detail: (i) ganglion mobilisation and fracture blocking during blowdown, and (ii) the mobilisation of trapped oil ganglia following surfactant injection.

Carbon Dioxide Migration in Permeable Cores: Characterizing and Controlling Flow for Geosequestration and Enhanced Oil Recovery

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ABSTRACT

Carbon dioxide (CO2) is a unique fluid, and controlling large scale injections of CO2 in the subsurface for geologic sequestration or enhanced oil recovery requires some novel techniques as well as a thorough understanding of how liquid or supercritical CO2 migrates through natural porous media. This presentation first discusses the difficulties in measuring CO2 saturation within cores under representative in-situ pressures and temperatures with computed tomography scanning, and describes some experimental and post-processing techniques. Variations in saturation as a function of sandstone properties and injection rates at elevated conditions are presented. A CO2 soluble surfactant is presented as a potential way of increasing the bulk viscosity (i.e. reducing the mobility) of the injected CO2 via the formation of CO2 in brine foams. Core scale experiments indicate an increase in pore occupation by CO2 when this surfactant is co-injected. This control of CO2 behavior could improve pore space utilization for sequestration, or assist in resource recovery within partially depleted oil reservoirs.

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CRYO-BIB-SEM to image Pore Morphology and Brine-Oil-Mineral Contacts in Carbonate Reservoirs

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ABSTRACT

Oil recovery is a complex process, largely depending on: (1) the exact fluid distribution in the rock's pore space, (2) the exact displacement process and (3) interfacial forces between the fluid phases and between fluids and the mineral surfaces. This affinity of fluids to be in contact with the rocks minerals is often referred to as wetting. Wetting phenomena are typically investigated by core flow experiments or by idealized contact angle measurements on flat mineral substrates. Both types of experiments have their strength and disadvantages since they are either not testing the real rock at the relevant length scale (contact angle measurements), or are testing the macroscopic displacement without insight into the exact displacement mechanism (core floods). Recently it has been shown that microscopic in-situ fluid-mineral configurations and contacts can be preserved by freezing and measured by cryo-Broad Ion Beam milling followed by cryo-Scanning Electron Microscopy (Cryo-BIB-SEM; Schmatz et al., 2015) with high resolution . In this study we aim to apply the same concept to carbonate rocks and with the goal to understand the influence of brine compositions on the microscopic fluid configurations and on production during water flooding.

Cryo-BIB-SEM in combination with EDX allows for directly studying the oil-water-mineral system in hydrocarbon-bearing reservoirs, at resolutions down to 5 nm (Schmatz et al., 2015). The technique allows for imaging of fluid-fluid-rock contacts at a resolution that permits testing of predictions on morphology and dynamics of fluid contact lines in relation mineral properties. Sub-micro effects on two phase flow, such as rugosity effects or thin water films separating the hydrophilic mineral surface from the oil, can be revealed with this technique and cannot be obtained by e.g., Micro-CT.

We quenched carbonate reservoir samples, which were saturated with oil and brine, to liquid nitrogen temperature and subsequently sectioned them using BIB-cutting under cryogenic conditions (Desbois et al., 2013; Schmatz et al. 2015). The flat cross-sections with dimensions of up to 4 mm2 allowed cryo-SEM imaging of oil-brine-mineral interfaces, with high-resolution EDX-mapping for phase identification. Prior to the in-situ experiments we quantified the pore structure (pore morphology, pore size distribution, mineral-phase related porosity) using BIB-SEM (Fig. 1, Norbisrath et al., 2015) and the pore connectivity by a combination of Wood's Metal injection and BIB-SEM (Klaver et al., 2015). These results will be complemented by pore structure information from gas physisorption data (N2 at 77K and CO2 at 273K) and mineral compositions from Rietveld quantitative phase analysis on X-ray diffraction patterns. The surface chemistry of the samples is assessed from dynamic vapor adsorption measurements with water and alkanes.

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Modelling the Transport of Wettability Modifiers at the Pore Scale

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ABSTRACT

Chemical treatments have been used in EOR processes to restore the wettability of bearing formations, improving the recovery factor and efficiency in the extraction process of hydrocarbons. Several models have been developed at the macroscopic scale for designing and predicting the behavior of wettability modifiers injected into the bearing formations. However, there is evidence of interactions between fluids and reservoir rocks, which are only deductible at the mesoscale and have a direct and emphatic effect on the recovery factor. Therefore, the development of pore scale models becomes the state-of-the-art of the optimization and design of chemical EOR processes.
In this work, we model and simulate the transport of wettability modifiers in heterogeneous porous media at the pore scale and their impact on multiphase flow properties (i.e. relative permeability, capillary pressure curves), in order to upscale and quantify the effect of wettability modifiers injection on the recovery factor at the macroscale. The multiphase RK Lattice-Boltzmann method was used in order to solve the Navier-Stokes and transport equations at the pore scale in 2D. Contact angle, surface and interfacial tension inherent to these systems are assumed to be affected by the local chemical concentration, which alters the wettability of the system. Several simulations were carried out to adjust LBM parameters with experimental data reported in the literature. Then, the impact of wettability modifiers injection was predicted in a macroscopic model using the relative permeability curves computed at the pore scale.
Finally, correlations between chemical concentration and reservoir properties (i.e. relative permeability curves, capillary pressure, residual oil saturation and capillary number) were obtained at the pore scale. As a result, the effectiveness of the treatment was found to be a function of the morphology of the system due to its heterogeneities and the solute mass transfer at the reactive fluid-fluid and fluid-solid interfaces. Thus, not only is the recovery factor dependent on the chemical local concentration, but also on the complex geometry of the system and phases distribution within the pores.

Increasing recovery factor in condensate-banking remediations using micellar dispersed in gas phase. a model approach

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ABSTRACT

Condensate banking is one of the most persistent formation damage mechanism in gas-condensate reservoirs. The liquid condensate is immobile by capillary and surface forces and creates a reduction on effective area to flux. To remedy this condition, a recent wellbore chemical stimulation technique was developed, named GaStim [SPE 152309, SPE 168133]. The technique is based on gas injection with dispersed stimulating fluid (micellar). To date, GaStim pilots have shown positive results in incremental oil production, showing that the gas phase as carrier fluid enables a better transport and mobilization of the chemical agent into the reservoir. However, the impact of chemical concentration, gas flow-rate, and other operative variables on the incremental production is unknown.

On other hand the technical/economic success or failure of the wellbore intervention depends on physical & chemical phenomena of micellar flooding into the reservoir. These phenomena include: micellar advective, diffusive and dispersive transport, mixing and dissolution of micellar with miscible phases, micro-emulsions generation, surfactant adsorption on matrix surface, surface and interfacial forces alteration, and others. Therefore, the understanding of underlying physical & chemical phenomena plays an important role in order to quantify the increased production. However the existing predictive models to quantify the incremental oil not include some relevant process as e.g. the dynamic adsorption. Therefore, an accurate modeling and simulation of the coupled transport and retention mechanism contributes to micellar deployment design that enables a major incremental oil production.

In this work, we develop a phenomenological model of the transport of a micellar carried by a gas phase in a reservoir with gas-condensate blockage. The model considers the micellar dissolution in the water and oil phases and the further adsorption on the matrix surface. The micellar transport equation considers the advective, molecular and diffusive transport mechanisms. Flow and transport equations are solved following the finite-volume method with a second-order discretization scheme. Transport and sorption requations are coupled to a multiphase/multicomponent reservoir simulator. The model predicts the evolution of micellar distribution in the reservoir in matrix and soluble phases. In addition, the oil recovery factor can be estimated for a given well intervention. The model was successfully validated with experimental data at lab-scale, showing an average agreement of 96%. Based on a previous pilot result, the model parameters were up-scaled from lab to reservoir scale. The model predicts the evolution of micellar distribution in the reservoir in matrix and soluble phases. In addition,

the oil recovery factor can be estimated for a given well intervention. The new model can be used for deployment optimization procedures in GaStim projects.

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On the Effect of Wettability, Hysteresis, and Spreading Films on Three-Phase Fluid Flow in Porous Media

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ABSTRACT

Enhanced oil recovery (EOR) strategies employing water-alternate-gas (WAG) injections may improve oil mobility and production recovery. WAG injections for EOR create regions in the reservoir with simultaneous flow of oil, water and air dominated by capillary and gravity forces. As a result of the dynamics in the transition zones, the invading fluid may snap off compartments of the displaced fluid which could then be trapped in the pore space, contributing to the hysteresis of the three-phase capillary pressure curves.

Three-phase capillary pressure curves are needed to model the three-phase transition zone movements in the reservoir. In reservoir simulation models, the common practice has been to implement three-phase capillary pressure curves based on two-phase gas-oil and oil-water capillary pressure data. However, experimental and modelling studies of three-phase fluid distributions at the pore scale have shown that this procedure is not always valid; three-phase capillary pressure curves exhibit hysteresis and depend on the saturation history of the three phases which cannot be derived from two-phase capillary pressure curves. Additionally, in three-phase systems, the fluid properties (interfacial tension) can dictate whether the system is conducive to the development of spreading films, which can have significant impact on flow and larger-scale applications (Blunt, 2001).

We have developed an experimental setup, compatible with x-ray computed micro-tomography, for three-phase fluid flow. The setup allows us to record capillary pressures while collecting high resolution 3D-image data of fluid distributions. We used this setup for drainage-imbibition experiments with brine, oil and gas – over wide range of saturations – in porous, glass-bead columns that were either uniformly water-wet or fractionally-wet (the latter using a mixture of water-wet and oil-wet beads). The 3D image-data, with a voxel resolution of 3.2 - 6.4 μm, were collected with synchrotron x-ray computed micro-tomography (CMT) at the GSECARS beam line 13-BM-D at the Advanced Photon Source, Argonne National Laboratory.

We present a quantitative comparison of the impact of the two wettability states, uniformly water-wet and fractionally oil-water wet, on the mobility, trapping and connectivity of the oil and gas fluid phases. In particular, we discuss how three-phase pore-scale mechanisms, such as oil layer existence and multiple displacement events, affect the mobility and trapping of oil in the porous medium. We also illustrate the impact of the two wettability states on the interfacial curvature of fluid-fluid interfaces as evaluated from the 3D image data (Li, 2015). The experimental data will also serve to develop, refine and confirm the simulation model developed by our collaborative partners.

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Microemulsion Formation of an EOR Surfactant

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ABSTRACT

In chemical enhanced oil recovery (cEOR) surfactant is added to the aqueous fluid injected into the reservoir. The presence of surfactant reduces the interfacial tension (IFT) between the oil and water phases by several orders of magnitude. The reduction in IFT is helps to mobilize the capillary trapped oil, but it is often accompanied by formation of a middle microemulsion phase. Consequently, the flow regime shifts from miscible to quasi-miscible. The oil recovery is largely affected by the displacement efficiency in this quasi-miscible regime, because the microemulsion becomes part of the flowing fluid system and it has to be recovered.
Microemulsion properties are typically studied using phase behavior tests at equilibrium conditions. However, under dynamic conditions, as in a reservoir system, the equilibrium state may never be reached. Here, we studied the microemulsion properties of an EOR surfactant with n-decane, under flow conditions in 2D glass microfluidic chips. The constitutive components, namely the surfactant solution and the oil phases, were co-injected via separate inlets into a T-junction where the initial mixing and formation of microemulsion phase occurred. The injection rates varied between 1 and 100 ft/day. A visualization method using a solvatochromatic Nile Red dye was developed; it allowed simultaneous visualization of all three phases (oil, water, and microemulsion) from a single image. The salinity of the surfactant solution, as well as the co-injection rates of the single components had an effect on the microemulsion formation and its flow properties. At low injection rates, slug flow occurred which then shifted to parallel flow as the injection rate increased.
Lastly, to substantiate the experimental observations, a numerical model was built to study the flow regimes during co-injection of two phases in a single capillary using COMSOL multi-phase physics module. Even though the model does not capture the effects of mixing or phase behavior to a full extent, the transition between different flow regimes were captured, and were consistent with experimental results.

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Complex interplay between wettability and shape factor defining the dynamics of entry capillary pressure of angular pores

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ABSTRACT

Entry capillary pressure of pores is one of the most important factors influencing the dynamics of multiphase flow in porous media and has a significant impact on many processes occurring in porous media such as remobilization of the capillary-trapped phases which is of great importance for the so-called enhanced oil recovery or soil remediation practices. Entry capillary pressure is controlled by several factors including the pore morphology, pore wettability as well as the flow dynamics.It is known that the entry capillary pressure is rate-dependent such that the inertia forces would enhance entry of the non-wetting phase into the pores. However, the concept of entry capillary pressure is mainly wettability-dependent. While the movement of a meniscus into a strongly water-wet pore is well-defined, the invasion of a meniscus into a weak water-wet pore and the role of pore geometry are unclear. In this study, using OpenFOAM (Open Field Operation and Manipulation) high-resolution pore-scale two-phase flow simulations have been conducted to expound the morphological time-evolution of the fluid-fluid interfaces as they advance through constricted angular pores. Drainage simulations have been done in simple pore geometries of square, equilateral triangle and irregular triangle at the capillary number (Ca) of 10-7 under different wetting conditions ranging from perfect to weak-wetting state where the advancement of interface through the angular pore becomes unstable. Under same wettability conditions, the interface is less stable as the poreshape factor(defined as the ratio of area to square of perimeter) decreases. Numerical results show that for the same wettability conditions angular pores with smaller shape factors induce enhancement of the meniscus movement that leads to smaller entry capillary pressure and non-linear temporal evolution of the entry capillary pressure. Our results offer new and fundamental insights regarding entry capillary pressure into pores; essential information for accurate description of flow in porous media.

The effect of pore wall texturing on multiphase flow in micro-models

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ABSTRACT

A number of recent studies [1] suggest that the wettability of the mineral surface is far more complex in real rock systems than most conventional models or measurements of wettability assume. Most models of multiphase flow in the subsurface assume a constant contact angle, based on simple contact angle studies of homogenous and polished surfaces. Recent in situ observation of these interfaces suggests that the predominant configuration involves a thin wetting layer separating the non-wetting phase from the mineral surface on either smooth or rough interfaces where the film fills the regions between surface asperities. This is important because a comparison of numerical simulations and experiments indicates a different dynamic evolution of drainage process noting that surface roughness or sticking effects can play a major role during multiphase flow [2]. Despite this, there is a fundamental lack of understanding with regard to the role of surface textures and dynamic flow conditions in multiphase flow through porous media.

A series of micromodel experiments were carried out to quantify the role of surface texture, fluid chemistry, and fluid flow conditions. Soda-lime glass capillaries were made with an average internal diameter of 500?m. Capillaries were either tested as received or treated in an aqueous solution of NaHCO3 for 24 hours at 120oC to create a nano-scale etching on the glass surface [3]. The etched capillaries were also cleaned with demineralized water and base piranha solution. A Nikon A1 confocal microscope was used to measure the speed, acceleration, and contact angle of the drainage and imbibition of Fluorinert and water. Experiments were conducted under various conditions, allowing the comparison of the dynamics of the flow between the smooth and the rough capillaries while controlling the rest of the parameter such as flow rate, interfacial tension and presence/absence of a water film. The results suggest that the role of pore wall texturing plays an important role on multiphase flow dynamics. An analysis of variance suggests the most statistically important factors in controlling the multiphase flow properties. Incorporating this effect to existing models will improve our predictive ability in multiphase flow problems.

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Formation of an emulsion in porous media and its properties

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ABSTRACT

Emulsification is helpful to oil recovery process, which is found to be a mechanism for EOR in alkaline flooding [1] and in alkaline-surfactant flooding [2]. However, there are a number of questions about conditions under which emulsification occurs, factors that influence the formation of emulsions, properties of naturally formed emulsions and so on.

It was found that emulsified water content of the oil/water mixture emerging from the porous medium was small at low injection rates, but above some threshold rate, the water content rose rapidly. The threshold rate depended on oil type, oil viscosity, water: oil ratio, permeability and wettability [3]. Oil phase capillary number, Nc', defined as (oil velocity) × (oil viscosity) / (oil-water IFT) was proposed to describe emulsification threshold [3]. The threshold Nc' increases with permeability of the medium and was significantly lower in oil-wet compared with water-wet sand.

The objective of this work is to study the effects of injection rate, flow distance, permeability and water: oil ratio on the formation of emulsion in porous media, and examine the conditions under which emulsions can form in situ and their properties.

Emulsification experiments are carried out using a range of sand packed tubes with length varied from 1.45m to 7.4m, average permeability varied from1170mD to 5380mD. Surfactant-alkaline solution (0.15wt% petroleum sulfonate and 0.1wt%NaOH, referred to as SA) and oil were injected simultaneously into a sand packed tube in a range of water: oil ratio and effluents are analyzed for emulsions' type, their droplet size distribution and emulsification ratio. Emulsification ratio is defined as Er, Er=Ve/ (Ve+Vo'), where, Ve is volume of effluent emulsions, Vo' is volume of effluent oil. Sand wettability is water-wet, model oil is used in which kerosene: Daqing dead oil ratio is 1:3, SA and oil viscosity is 0.7 mPa.s and 10 mPa.s, oil-SA interfacial tension is 1.95 mN/m. The injection rate varies from 3.47×10-5 m/s to 4.17×10-4 m/s.

Emulsification dynamic parameter is proposed to evaluate the comprehensive effects of injection rate (v), flow distance (L) and permeability (K) on formation of emulsion and to describe emulsification threshold, defined as Em= vL/K. Emulsification threshold is Emc. Lower than Emc, no emulsification takes place; equal to or greater than Emc, with the increase of Em, Er increases firstly and then decreases (Figure 1). The ratio of water to oil has significant influence on Em, the higher the percentage of oil volume, the greater Em. The experimental results also showed that size and size distribution of naturally formed droplet can adjust during flow in porous media and gradually match with pore size and pore size distribution. Within emulsification occurrence region, the average diameter of most of droplets (Dd) is about 3~5 times the diameter of most of pore throats (Dt) (Figure 2).

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Mathematical Modeling of Combined Chemical-Thermal EOR Methods

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ABSTRACT

The injection of hot water containing surfactant is an Enhanced Oil Recovery (EOR) process that can increase both the volumetric sweep efficiency and displacement efficiency and is referred as a combined thermal-chemical method. In this presentation, the one-dimensional three-phase flow of oil displacement by hot water containing dissolved surfactant in reservoirs is analyzed. It is considered that the surfactant may be dissolved in water and oil phases and also be adsorbed by the rock.
The system is investigated through three different cases in order to examine the effects of surfactant adsorption and its partitioning between water and oil phases: Case A, considering only the surfactant partitioning, Case B, considering only surfactant adsorption, and Case C, considering both partitioning and adsorption. The cases that take the surfactant adsorption into account are modeled by two different adsorption isotherms: Langmuir and Freundlich.
The system is described by a hyperbolic system composed by three equations: the energy conservation, the water mass balance and the surfactant mass balance, which can include the partitioning between the water and oil phases and its adsorption by the rock, thus depending on the adsorption isotherm. We considered the continuous injection case, the injected fluid temperature is greater than the reservoir temperature, and that initially there is no surfactant dissolved in the oil and adsorbed by the rock. The solution was obtained using the Method of Characteristics.
The solutions show the effect of the adsorption on each case: when adsorption is neglected, the surfactant concentration shock wave velocity is higher than the temperature shock wave velocity; when adsorption was considered, the opposite occurred. If the adsorption model follows the Langmuir isotherm, the solution of the hyperbolic system results in a shock wave for the surfactant concentration, if the solid-liquid equilibrium is based on the Freundlich isotherm, then a rarefaction wave for the surfactant concentration appears in the solution. The temperature transition between two fractional flow functions is always a shock. The water saturation profile is composed by a rarefaction wave at constant temperature and surfactant concentration, then a shock wave following the temperature transition, a rarefaction wave or a shock wave depending on the type of adsorption isotherm and finally a Buckley-Leverett type shock. The solution is constructed in the fractional flow function space, outlining the shock and rarefaction regions. The behavior of the recovery factors versus dimensionless time shows the differences related to each adsorption isotherm during the production of a field submitted to this enhanced oil recovery technique. The analytical results obtained were compared to numerical simulations and presented close agreement. These results show the importance of laboratory experiments in the production forecast.
The application of the developed analytical method allows the modeling of combined thermal-chemical enhanced oil recovery methods. Depending on the solid-liquid equilibria, which should be obtained in the laboratory, a different surfactant concentration behavior will be developed in the reservoir. The expected recovery factor evolution with time shows the importance of the choice of the proper thermodynamics model.

Application of Fractional Flow Theory to Composite Media in EOR Processes

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ABSTRACT

Fractional flow theory is a simple and powerful tool for the development of analytical solutions to characterize enhanced oil recovery processes. This approach provides a quick and easy way to predict important features of the recovery method. However, this theory is based on the assumption that the porous media is homogeneous, i.e., the rock and fluid properties do not change over space.
In this work, we extend the fractional flow theory to enhanced oil recovery processes, in particular the chemical methods, considering the porous media composed by two regions with different porosity, relative permeability and adsorption curves. The extension of this technique to other EOR methods, like thermal and miscible, is straightforward. The proposed solution is formed by rarefaction and shock waves besides constant states. The structure of the solution depends on the relative position of the fractional flow curves. The main difference between the homogeneous and the presented solution is that after the polymer shock front crosses the interface that separates the two regions a rarefaction wave appears at the displacement front. In some cases the velocity of this front might increase over time.
The solution was compared to a numeric reservoir simulator based on the finite difference method, which does not capture the shock waves precisely. The solutions presented in this work can be used to validate numerical methods, to obtain parameters of laboratory experiments, and to be used in streamlines reservoir simulators. This methodology can be extended to porous media composed by N regions.

Pore-scale Investigation of Solvent Based Bitumen Recovery

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ABSTRACT

This study investigates oil displacement mechanisms during solvent based extraction methods, specifically non-condensing and condensing solvent extraction using a glass micromodel. Microfluidic platforms allow direct visualization and rapid evaluation of pore-scale recovery mechanisms associated with various EOR processes. A microfluidic model with compact posts of 140 ?m in diameter were etched on a 10cm × 10cm glass to construct a 2D porous medium, which had pore characteristics in the range of oil sand formations. The chip was initially filled with Athabasca bitumen and thereafter, light hydrocarbon solvent was injected at various temperatures (25–100 °C) and pressures (400–1900 kPa) to produce the bitumen. A DSLR camera (Nikon D3300) was used to capture time-lapse images during the entire process. Different mechanisms at the pore-scale were observed via utilizing a digital microscope (Dino LITE). The images were then analyzed for the pore-scale analysis and interface behaviours.

Two types of interface were observed during the runs and the phase of solvents determined the pore-scale mechanisms at the interface. For non-condensing solvent extraction, the solvents remained in vapour phase for the entire run and the bitumen viscosity was lowered as a result of dissolution of solvent vapour into bitumen. Associated pore-scale mechanisms were observed, such as “snap-off”, “bubble entrapment”, and “trailing pore advancement” [1]. During condensing solvent extraction process, the solvents are heated and pressurized so that they would condense upon contact with the cold bitumen front and the bitumen viscosity subsequently reduces through both heat transfer and mass transfer. It was observed that a second chamber was formed after the vapour chamber as the solvents completely condensed into liquid. Several differences were found between the two chambers. Liquid solvent has a much worse sweeping efficiency than vapour solvent and left a large amount of residual bitumen in the pores. Also, the liquid solvent and bitumen interface, seemed to be less dynamic compared with the vapour solvent and bitumen interface. Bitumen dilution could be observed at the interface where the bitumen became lighter and lighter in colour over time. Furthermore, asphaltene precipitation observed in the pores in swept regions, particularly in the vapour chamber. Overall, the condensing solvent extraction process creates a much more complicated system than the non-condensing solvent extraction process and bright-field images are not sufficient to study the pore-scale phenomena during the the condensing solvent extraction process. The next step is to incorporate fluorescence microscopy to differentiate the phases in the system during the process in order to capture the dynamic of bitumen dilution and asphaltene precipitation in the pores at the interface. Three images are submitted with the abstract. The first image demonstrates the run

conditions of the condensing solvent extraction process and non-condensing solvent extraction process. The second image shows the pore-scale mechanisms observed in the non-condensing solvent extraction process, while the last image demonstrates displacement mechanisms in the condensing solvent extraction runs.

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A STUDY ON COUNTER – CURRENT IMBIBITION PHENOMENON ARISING IN FLUID FLOW THROUGH POROUS MEDIA WITH INCLINATION AND GRAVITATIONAL EFFECT

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ABSTRACT

Counter–current imbibition, where water spontaneously enters a water-wet rock while oil escapes by flowing in the opposite direction is a key recovery mechanism in oil reservoirs. In this paper, it discusses the counter–current imbibition phenomena in Homogeneous porous media with inclination and gravitational effects calculate the saturation rate of wetting phase by using Adomian decomposition method. This problem has a great importance in the oil recovery process.

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Simplified Numerical Model of Surfactant-Polymer (SP) Flooding Process in Porous Media for Enhanced Oil Recovery

Presenter: Seyed Mojtaba Hosseini Nasab
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ABSTRACT

Surfactant-Polymer flooding process could significantly enhance oil recovery from water flooded oil reservoirs through synergetic effects of creating mobility control of the displacing fluid, reducing interfacial tension forces between water/oil phases and inducing a wettability alteration. In this paper, we present the simple physical based numerical model that simulates SP flooding process for enhanced oil recovery (EOR). In this study volume fraction balance for black-oil subsystems was selected for developing numerical model. The model was upgraded by taking into account different aspects of SP EOR process such as gravity effect, capillary pressure, mobility reduction factor, polymer/surfactant adsorption and interfacial tension (IFT) reduction between water/oil phases. The Langmuir isotherm coefficients for adsorption of polymer and surfactant were used from separately laboratory experiments of single component injection of surfactant and polymer in the Bentheimer sandstone core. The systems of equations were solved in the Finite Elements based Method (FEM). The validity of the implementation was tested by comparing the results attained from simplified numerical model with laboratory core-flooding experimental data of SP flood into Bentheimer sandstone core. A comparison showed excellent agreement between the numerical results with the experimental investigations in this work. This confirms the numerical model developed in this work is robust and has capability to reproduce the main features of high viscosity surfactant flooding (SP) EOR in the consolidated sandstone porous media. A subsequent analysis on the effect of several parameters including permeability, mobility reduction factor, polymer/surfactant adsorption and IFT on the efficiency of SP flood oil recovery was conducted by the validated numerical model.

Modelling moisture evolution and transient sorption behavior of paperboard using hybrid mixture theory

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ABSTRACT

To be able to adapt and develop new competitive paperboard packages it is necessary to understand the material behaviour throughout the different stages of the product life. Here paperboard is seen as a porous media consisting of a network of wood fibers with pores filled with moist air and water. The fibers have a high affinity towards water, thus water vapor is readily adsorbed from the environment. Similarly liquid water is absorbed by the fibers if the material is not chemically treated to become hydrophobic. The presence of water in the fibers strongly influence the mechanical properties of the board and is therefore important in many paperboard applications, such as storage of paperboard rolls and sterilization of food packages.
In this work Hybrid Mixture Theory framework is adopted to derive a thermodynamically consistent material model for transport of moist air and water as well as mass exchange between vapor and bound water. Mixture Theory balance laws for mass, linear momentum and energy are established for each constituent [1]. The dissipation inequality is derived in the same fashion as in the work by Bennethum and Cushman [2], Ristinmaa et al. [3] and is used to derive the macroscale constitutive relations. The sorption behavior of the material which is an important part of the coupling between the temperature, moisture and humidity are described by the water activity and enters the description of the chemical potential [4].
The paperboard model is used to simulate the moisture evolution and transient sorption behavior of the material, subjected to different environments.

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Vapor transport in a porous smectite clay: from normal to anomalous diffusion

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ABSTRACT

Smectite clays are widely found on the Earth surface. They are porous materials possessing connected mesopores in the micrometer range, in-between mineral grains, and nanopores inside the grains. These grains are stacks of individual 1 nm-thick clay particles (the layers) and have the ability to swell by incorporating H2O molecules (or other molecules such as CO2) in-between the layers, depending on the ambiant temperature and on the humidity present in the mesopores surrounding the grain. Imposing a gradient of relative humidity H along a temperature- controlled dry sample of smectite clay, we investigate the diffusive transport of water molecules in vapor phase through the material. As water molecules diffuse through the mesopores, some of them intercalate into the nanopores, causing the grains to swell and therefore a decrease in the mesoporous volume available for vapor diffusion. These two effects render the transport process potentially anomalous; we monitor it using space- and time-resolved X-ray diffraction at a synchrotron source. Indeed, water absorption into the nano-layered grains changes the interlayer repetition distance (d-spacing) of the stacks, which is seen as a horizontal translation of a peak in the diffraction data. A calibration experiment performed under controlled constant temperature and controlled humidity level all around the sample, varying H by steps, has allowed us to map the monotonous evolution of d as a function of H. By mapping d in space and time in the transport experiments we thus obtain humidity H(x) profiles along the direction of the initial humidity gradient, at regular time intervals t. To model the data we consider a one-dimensional effective diffusion process described by a fractional time diffusion equation with a diffusion coefficient that depends on humidity. It is possible to rescale all humidity profiles onto a single master curve as a function of (x/t)?/2, where ? is the exponent characteristic of the fractional derivative. We observe that when the clay sample is prepared with sodium cations intercalated in the nano-pores, vapor transport is normal (?=2), while if the interlayer cation is lithium the transport is strongly subdiffusive. We explain this behavior by the very different time scales observed in the intercalation dynamics of the two cations. The mechanism at play is reminiscent of retardation mechanisms known in other subsurface media, but with a nanoscale trapping mechanism and a feedback effect of the mesoporous humidity on the local porosity of the medium. In both cases we also obtain the dependence of the effective diffusion coefficient on humidity.

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Modeling Vapor Transport through Partially Saturated Porous Media at the Pore Scale Using Chemical Potential

Presenter: Lynn Schreyer
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ABSTRACT

Modeling vapour transport through partially saturated porous media is complicated due to the interactions at the microscale and the coupling between the interactions between the solid, liquid, and vapor phases. The traditional approach to modelling porous media uses concentration, pressure, and saturation as the primary dependent variables. Here we introduce chemical potential as an alternate dependent variable and show that it simplifies conceptually and mathematically the modeling of vapor transport. In this talk we revisit the fundamentals of chemical potential, provide a simple one-dimensional pore-scale model, and compare the model with experimental results.

Homogenous drying of nano-porous media during the falling rate period

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ABSTRACT

Drying of a wet coarse grain packing or more generally a wet porous media, is a well known process in which the desiccation rate exhibits 2 main regimes. Firstly, a constant rate period (CRP) takes place where the material desaturates in a homogeneous way involving a well-known capillary equilibration process that implies substitution of liquid water by vapor-saturated air. Further drying triggers a falling rate period (FRP) during which a dry front is seen to grow from the free surface. In this situation, the drying kinetics is seen to correspond to diffusion of vapor from the wet front located in the sample, towards the free surface and through the porous structure. This process was observed with micro or macroscopic porous media but we do not know if it occurs in a similar way in nano-porous materials.

Using highly resolved H proton Magnetic resonance Imaging profiling to spatially locate the water in the sample along the Z axis in a variety of porous structures (made of monodisperse beads with pore size ranging from 45 microns to few nanometers) shows that it exists a critical pore size under which the above situation is not valid anymore. For small enough pores no dry front is seen to develop but rather a slight gradient of water saturation is observed throughout the sample in the FRP [1]. Paradoxically, the drying rate during this period still scales as the square root of time whereas there is no dry front progressing in the sample. We show that this result from the Kelvin effect: when the radius of curvature is sufficiently small vapor at a density smaller than the maximum value can coexist with a liquid interface at this temperature so that a gradient of vapor density can exist throughout the wet sample.

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Development of a fully coupled thermo-hydro-mechanical-chemical simulator for gas hydrate extraction

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ABSTRACT

A fully coupled thermo-hydro-mechanical-chemical model has been developed for the wellbore stability analysis during drilling the hydrate bearing sediments. Within this model, the phase change from hydrate to fluids, the flow of pore water and gas, the mechanical behavior of the solid skeleton, and heat transfer can all be simultaneously solved. The mechanical behaviour of sediment is modelled as poro-elasto-plastic, and the failure condition is represented by a modified Mohr Coulomb yield criterion.
Taking advantage of the finite element scheme with an adaptive relaxed Picard method, the proposed model is implemeted into a robust simulator named PorousTH2MC. By using this simulator, the dissociation process induced by drilling through hydrate-bearing formation is analyzed. Results show the the evloution of temprature, gas pressure,water pressure, displacements and plastic zone around the wellbore during hydrate dissociation. The developed numerical model is found to be very useful in predicting the responses of hydrate bearing sediment.

Multiphase CO2 Migration Through Shallow Aquifers During Leakage From Geologic Carbon Sequestration Sites: Comparing an Equilibrium-Based Numerical Code Against Intermediate-Scale Experimental Data

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ABSTRACT

In order to assess the potential risks of Geologic Carbon Sequestration (GCS) activities, it is crucial to understand the fundamental processes that are likely to occur if and when stored carbon dioxide (CO2) leaks upward from a GCS site into the shallow subsurface. The potential risks of CO2 leakage include degradation of groundwater quality by dissolution of CO2, as well as escape of gas phase CO2 to the atmosphere through exsolution and gas migration. Intermediate-scale laboratory experiments and numerical models allow for improved understanding of these complexly interrelated processes, because the boundary conditions, initial conditions, and porous media parameters can be better controlled and observed in the laboratory than in the field. Previous experimental and numerical works [1]–[5] have identified several factors that control the exsolution, accumulation, and flow of CO2 gas in water saturated, one dimensional porous media systems containing various types of heterogeneities. The goals of this work are: (1) to upscale the findings of those studies into more realistic, two dimensional (2-D) systems by gathering high-resolution data from a large experimental test system, and (2) to assess the capability of an existing multiphase flow simulator to capture the behaviour observed in the experiments.

For this study, a large 2-D test system was constructed, densely instrumented, and filled with sand and water to mimic a shallow aquifer with layers of different porous media. As clean water flowed across the system due to an imposed head gradient, a separate stream of water was infused with dissolved CO2 and injected into a port at the bottom of the system. A total of 97 soil moisture sensors were strategically placed throughout the system to monitor the evolution of the gas phase CO2 plume through time. Aqueous samples were taken from a grid of ports and analysed with an Ion Chromatograph to monitor the flow of dissolved CO2. The small amount of headspace at the top of the system was separated into four components, each of which was connected to a gas flow meter to continuously monitor the outflow of gas phase CO2 to the atmosphere. Two different sand combinations were used in separate experiments in order to assess the relative effects of different types of heterogeneities on the CO2 transport through the system.

Results from the experiments were then compared to simulations performed with the Finite Element Heat and Mass Transfer (FEHM) code from Los Alamos National Laboratory. After minimal adjustments of the important parameters and conditions, the model was able to accurately capture some, but not all, of the CO2 evolution processes. This indicates that FEHM is potentially useful for predicting CO2 migration through the shallow subsurface in some instances of CO2 leakage, but that

the local equilibrium assumption upon which the code operates may potentially limit its application in some cases or at some scales.

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Laboratory study of plant-soil-atmospheric interactions and vegetation distribution in water limited arid environments using a coupled porous media-climate controlled wind tunnel

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ABSTRACT

Evapotranspiration and bare-soil evaporation are critical components of hydrologic mass balances, accounting for a significant portion of total water fluxes from the land to the atmosphere. The water essential for supporting plant growth is drawn via capillary gradients established between the root zone and the surrounding bulk soil. Plant distribution and density over a landscape is governed necessarily by the availability of water; individual plants must compete for the same soil water limited by climate and soil conditions. In a previous study, the authors investigated the impacts of coupled atmosphere–bulk soil–vegetation interactions on shallow subsurface soil moisture dynamics in the vicinity of a single simulated plant under strictly drying conditions. Results demonstrated that the soil moisture is controlled to varying degrees by both the root zone and the physical structure of the vegetative canopy. This experimental and numerical study expands on our previous work by investigating how interactions between two plants, specifically their competition for water, effect local soil moisture dynamics. Experimentation is performed in the fully instrumented intermediate scale porous media-wind tunnel test facility at the Center for Experimental Study of Subsurface Environmental Processes (CESEP) at the Colorado School of Mines. Limestone blocks are used as analogs for real plants in order to reduce the complexity of the system (e.g. plant growth, irregular geometry, canopy flow) while still maintaining water suction similar to that of natural root zones and providing evaporative surfaces similar to leaves. Results show that the soil moisture dynamics in the presence of two plants (i.e. limestone blocks) is very different than that of a single plant. The physical spacing between the two blocks determines their degree of influence or interaction with each other in terms of both water availability and changes in local atmospheric conditions. This work can provide new insights into observed plant behavior (i.e. growth rate, spacing patterns, density) in sparsely vegetated arid or semiarid environments where water availability is limited and demand is high.

Water Vapor Transport in Porous Media Estimated by Heat Flux Theory

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ABSTRACT

Water vapor transport in porous media was investigated by Philip and de Vries (1957), and Fick's law was proposed to govern the phenomenon. They found discrepancy between experimental observation and theoretical estimation, where the former values were significantly larger than those estimated by theoretical equation. The under estimation of theoretical equation was resolved by introducing water vapor enhancement factor. Soil physics community had been using this factor for more than 50 years, and efforts were carried out to better understanding the underlying phenomenon. The work of Cass et al. (1984) had made significant contribution in providing both experimental solution and theoretical framework in estimating water vapor enhancement factor. Cass work was commonly compared to the work of Cary (1965) who had estimated phenomenological enhancement factor, which is comparable to water vapor enhancement factor by a simple mathematical equation. Their works had proven the presence of water vapor enhancement in porous media, and subsequently Ho and Webb (1999); hence, it had suggested the presence of at least an unknown phenomenon that was yet to discover. In this study, we re-examined the theoretical framework of heat flux theory that was used by Cass et al. (1984) to estimate water vapor enhancement factor. Then, we proposed improvement to the heat flux theory based on the work of de Vries (1958). Subsequently, we utilized the experimental data of Cass et al. (1984) and investigated with the improved heat flux theory to estimate the water vapor enhancement factor. The theoretical explanation of Parlange et al. (1998), i.e. the expansion and contraction of air due to temperature variation, was utilized as the basis to introduce water vapor advection term, i.e. Darcy's law, that the variation of temperature was in relation to the combined water vapor pressure and water vapor density, as governed by the ideal gas law. The possibility of using advection equation to governed water vapor enhancement factor was first described by Ho and Webb (1996), but it was not tested. In the new theoretical framework, water vapor enhancement factor was detached from the Fick's law transport equation to create a new term for water vapor advection. A considerable details of the advection equation was described as in Ho and Webb (1999), except an empirical mathematical equation that was introduced in this study to govern the water vapor relative permeability that was resulted by water vapor vaporization (volume expansion) due to temperature, without the presence of external pressure force. In combination of the gas slipping effect from Klinkenberg (1941) and the newly proposed relative permeability, the results had showed that the proposed mathematical solution was in good agreement with the trend of experimental data from Cass et al. (1984).

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Mathematical modeling of gas migration pathways affected by subsurface and climate factors.

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ABSTRACT

The intrusion of vapor from trapped non-aqueous phase liquid contaminant sources and dissolved chemical plumes into subsurface structures and buildings has received attention due to the potential health risk to their occupants. Both field and laboratory investigations have identified source conditions, subsurface geologic heterogeneity, climate conditions and other building specific features contribute to the variation concentrations from building to building as well as temporal changes within each building. Numerical models are useful in the complete analysis of these factors and their interactions to interpret monitoring data, make the assessment of potential risks and evaluate corrective action. Early models used for vapor intrusion analysis assumed steady conditions, thus limiting their use in most practical situations. A few transient models have been developed to represent some of the factors that contribute to the spatial and temporal variability of the concentration measurements. However, these models have not incorporated all the complex interactions of the subsurface and atmospheric systems to analyze how the climate drivers affect the vapor intrusion pathways. Past experimental data from an intermediate scale experiments demonstrated the development of dynamic air pathways due to soil moisture variability in the subsurface affected by the land surface boundary conditions. The development of a model that captures the subsurface and source conditions, and the climate drivers such as rainfall and capping due to high soil moisture buildup at the land surface that affects the air pathway development is presented. The developed model is based on mixed-hybrid finite element method. The model was used to simulate a set of hypothetical scenarios to demonstrate the model capabilities and sensitivity of climate to transient vapor concentrations in a building. The model will be further developed and validated using experimental data.

Multiscale Modeling and Experimental Verification of Water, Vapor and Heat Transport in Expanding Starch Matrix During Extrusion

Presenter: Pawan Takhar
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ABSTRACT

Water, vapor and heat transport mechanisms and thermomechanical changes occurring inside the expanding starch extrudate were described using the hybrid mixture theory based unsaturated transport equations. Transport equations were transformed from the Eulerian coordinates to the Lagrangian coordinates. Good agreements between the predicted and the experimental values of surface temperature, moisture content and expansion ratio of the extrudates were obtained. The model was also used to calculate temperature, moisture content, pore-pressure and viscoelastic-stress distribution in the extrudate. Matrix collapse and glassy crust formation under the surface was calculated as a function of extrusion conditions. Expansion behavior of the extrudate was described using the difference between the stress due to pore pressure and viscoelastic stress. The modeling results can serve as a guide for predictably modifying the extrusion parameters for obtaining specific textural attributes of expanded starch for various food, feed and biomedical applications.

Neutron Scattering Characterization of Confined Fluids

Presenter: Yuri Melnichenko
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ABSTRACT

Fluid-solid interactions in natural and engineered porous solids underlie variety of technological processes, including carbon capture and sequestration, hydrogen storage, membrane separation, and catalysis. The size, distribution and interconnectivity of pores, the chemical and physical properties of the solid and fluid phases collectively dictate how fluid molecules migrate into and through the micro- and mesoporous media, adsorb and ultimately react with the solid surfaces. Due to the high penetration power and relatively short wavelength of neutrons, small-angle neutron scattering (SANS) is ideally suited for in situ studies of the structure and dynamics of confined fluids as well as for evaluating structure of pores in engineered and natural porous systems. In this talk I will overview some recent developments in the SANS methodology and give several examples of how it can be used for in-situ studies of the adsorption of carbon dioxide in porous silica and activated carbon as well as characterization of the abnormal densification of fluids in sub-nanometer pores at ambient temperatures [1].

[1] Y. B. Melnichenko, Small-Angle Scattering from Confined and Interfacial Fluids. Applications to Energy Storage and Environmental Science, Springer, 2015.

Structural and thermodynamic studies on the phase behavior of water in ordered mesoporous host structures with different pore sizes and different surface polarities

Presenter: Michael Froeba
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ABSTRACT

In a first step on the way to study the structural and thermodynamic behavior of water in ordered nanoporous structures the respective host materials were synthesized. Several mesoporous silicas and organosilicas (PMOs) of the MCM-41-type with a narrow pore size distribution were synthesized using the liquid-crystal template approach with ionic surfactants as structure-directing agents (SDAs). The obtained pore diameters were in the range between 2 and 5 nm. In contrast to the pristine silica the PMOs contain organic bridging units (SiO1.5-R-SiO1.5) within the quasi-crystalline pore walls. The organic units R used were ethane, benzene, aniline 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 70 %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 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- and biphenylene-bridged PMOs exhibit a quasi-crystalline long range order. Due to this there are two different regions in the pore wall which lead to a regular modulation of the surface polarity in the direction of the pore channel. 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 in close proximity to the inorganic regions of the pore wall than to the organic because of the different surface polarities.

Investigation of local pore structure and sorption induced deformation in hierarchical mesoporous silica by nanobeam X-ray diffraction

Presenter: Lukas Ludescher
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AUTHORS

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ABSTRACT

In this study we aim at measuring the local sorption induced deformation of differently tempered hierarchically organized (meso)porous silica upon the change of relative humidity (RH). The material consists of an interconnected macroporous network of 1-2 µm long struts with roughly 300 to 500 nm diameter comprising hexagonally packed cylindrical mesopores [1]. Joints forming at the points where the struts meet are expected to exhibit different deformation behaviour from the struts themselves, and thus, to significantly influence the macroscopic sorption deformation. Two samples calcined at 500 °C or tempered at 750°C, respectively, were used to prepare isolated struts or strut/joint agglomerates on amorphous Si3N4 membranes. Small angle X-ray diffraction (SAXS) using a 150 nm pencil X-ray beam was employed at the nanofocus branch of the microfocus beamline ID13 of the European Synchrotron Radiation Facility ESRF. Figure [1c] shows 2D diffraction patterns on a 2D mesh scan across a single strut/joint agglomerate.The difference in humidity was achieved via a specialised set-up in a flow-cell under an adjustable stream of humidified nitrogen. Local resolution is defined by the beam diameter, which was adjusted to circa 150 nm. The local strain was determined from the position of the [10] reflection of the pore lattice by repeatedly scanning the sample across the nanofocused beam followed by change of relative humidity. Hence, we obtain 2D strain maps not only on the strut itself, but also on the yet not fully understood joint regions. The information gained from this experiment is expected to contribute to a better understanding of the complex poromechanics in such systems, thus allowing to further develop and refine current theoretical approaches [2].

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Methane Adsorption in Model Porous Materials Studied by Small-Angle Neutron Scattering

Presenter: Wei-Shan Chiang
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ABSTRACT

Over the past decade, shale gas production significantly increases in the United States. The adsorption properties of natural gas highly influence the gas transportation in shales and the estimation of total shale gas in place (GIP). These properties closely relate to the size and surface properties of shale nanopores. In this study, adsorption behavior of methane onto the surface of model mesoporous materials, SBA-15 and MCM-41, is investigated by small-angle neutron scattering (SANS). A new scattering model is developed to investigate the gas adsorption behaviors at a wide temperature range at ambient pressure. Detailed structure determination of gas adsorption is achieved by the model fitting. The adsorption layer thickness and the excess adsorption are extracted above capillary condensation temperature Tc. The liquid and solid methane density are determined using the SANS data at the temperature below Tc. The surface roughness is found to play a very important role for the gas adsorption. However, the proposed models of density profile for gas adsorbed on the solid matrix in literatures are insufficient to explain our scattering data. These results are important for us to eventually understand methane gas adsorption in nanometer-sized pores, which are abundant in shale rocks, at high temperatures and high pressures.

Insights from plants: evaporation-induced nanoflows

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ABSTRACT

Moving fluids at the nanoscale is a difficult process due to massive viscous friction, and requires very large driving forces, which can be inconvenient and costly.
Inspired by plants, we used evaporation to generate controlled, steady-state flows in pores ~3-nm in diameter embedded in a silicon-based microfluidic system. The capillary pressures that drives the flow (tensions on the order of tens to hundreds of MPa in magnitude) develop spontaneously upon drying and can be externally tuned by changing the relative humidity (vapor saturation) outside of the sample.
We will show that the analysis of the dynamic drying response allows for the investigation of both thermodynamic and fluid-mechanical aspects of the physics of the fluid in the nanopores. We find excellent agreement with predictions from macroscopic, continuum-based theories (Kelvin equation, Capillary-viscous flows) provided that the hydrodynamic radius of the pores is reduced by a single monolayer of fluid molecules adsorbed at the pore wall.
Beyond providing new dynamic methods for investigating the fundamental physics of fluids at the nanoscale, our results also suggest ideas for handling liquids in controlled ways for lab-on-chip and microsensor applications. We will finish by briefly discussing flow enhancement possibilities based on ideas from the vascular anatomy of plants.

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Hydraulic Transport Across Hydrophilic and Hydrophobic Nanopores: Flow Experiments with Water and n-Hexane

Presenter: Patrick Huber
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ABSTRACT

We experimentally explore pressure-driven flow of water and n-hexane across nanoporous silica (Vycor glass monoliths with 7 or 10 nm pore diameters, respectively) as a function of temperature and surface functionalization (native and silanized glass surfaces). Hydraulic flow rates are measured by applying hydrostatic pressures via inert gases (argon and helium, pressurized up to 70 bar) on the upstream side in a capacitor-based membrane permeability setup. For the native, hydrophilic silica walls, the measured hydraulic permeabilities can be quantitatively accounted for by bulk fluidity provided we assume a sticking boundary layer, i.e. a negative velocity slip length of molecular dimensions. The thickness of this boundary layer is discussed with regard to previous capillarity-driven flow experiments (spontaneous imbibition) and with regard to velocity slippage at the pore walls resulting from dissolved gas. Water flow across the silanized, hydrophobic nanopores is blocked up to a hydrostatic pressure of at least 70 bar. The absence of a sticking boundary layer quantitatively accounts for an enhanced n-hexane permeability in the hydrophobic compared to the hydrophilic nanopores (1,2).

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Core-shell tubular structures of binary liquids confined in cylindrical nanopores

Presenter: Denis Morineau
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ABSTRACT

The properties of liquids confined in nanometric cavities can be very different from their bulk counterparts, which raises exciting new questions for basic condensed matter physics. Among many fascinating confinement effects, we focus on the formation of new liquid structures of binary systems confined in nanochannels
Glassforming H-bonding liquids are especially interesting candidates because of their tendency to develop both supramolecular order and cooperative dynamics, which might be particularly sensitive to confinement at the nanoscale. Indeed it is striking that the ability of alcohols to spontaneously form mesoscopic ordered structures could be tuned, either by dispersion in an aprotic solvent [1], or by confinement in porous silicates [2-4].
We will discuss how this study went one step further recently, with the observation of confinement induced micro-phase separation of fully miscible tert-Butanol/Toluene binary mixtures confined in different types of straight, mono-disperse, rigid channels of mesoporous MCM-41 and SBA-15 silicates (D = 3.5, 7 nm).
Neutron diffraction experiments with selective isotopic compositions have been performed to vary systematically the scattering length density of the different compounds. It resulted an apparently anomalous modulation of the intensity of the Bragg peaks of the mesoporous system, which demonstrates that the liquids are really inhomogeneous at the nanoscale. We have derived a core-shell model whose predictions rationalize the experimental observations. It shows the existence of a micro-phase-separated tubular structure with the segregation of alcohol that forms a layer at the pore surface, which surrounds a rich-apolar solvent core.
We addressed the molecular relaxations at play on the different timescales that govern the individual molecular dynamics of the segregated components on one hand, and the glass transition of the whole binary system on the other hand by dynamical studies (Quasielastic Neutron Scattering, Dielectric Spectroscopy, and modulated Calorimetry).
This core-shell phenomenon is probably more general. We believe it is related to different interfacial interactions that have been quantified by Dynamical Vapor Sorption experiments: a situation which is awaited for a variety of other complex fluids in nanopores

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Interpretation of the phase composition curves of frozen soils via molecular dynamics

Presenter: Zhen Liu
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ABSTRACT

The phase composition behavior of frozen soils is a fundamental relationship in understanding permafrost and seasonally-frozen soils and thus of great interest in cold regions engineering. However, due to the complex interplay of adsorption and capillary effects, a clear physically-based understanding of the phase composition curves in the low temperature range is still absent. Especially, it is unclear whether the Young-Laplace equation corresponding to capillary still holds in nano-scale pores where adsorption could dominate. This paper employs molecular dynamics simulation to investigate factors that can possibly influence the complex physical process underlying the freezing of pore water. A monoatomic water model was adopted to depict interatomic potentials while a cylindrical nanopore with a face-centered cubic crystal structure was selected to represent the nano-size pores perforating the mineral matrix. The wettability of the nanopore was controlled by adjusting the water-nanopore interaction energy. A specific simulation procedure was presented for the determination of the melting temperature. A series of simulations was conducted to unravel the effects of the pore size and wettability on the freezing of pore water. It is observed that the melting temperature decreases slightly with the increase of nanopore wettability. Besides, the water confined in nanpores with a diameter of 1 nm and 2 nm could not form an effective ice crystal structure due to the molecular order caused by the dominant adsorption effect. The simulated melting temperatures of ice confined in nanopores with a diameter of 3 nm, 4 nm, 5 nm and 6 nm are 20-24 K lower than those predicted using the Young-Laplace equation. It is therefore concluded that the adsorption effect may be significant in the low temperature range corresponding to nano-scale pores.

Behavior of C-O-H Fluids in Nanopores

Presenter: David Cole
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ABSTRACT

Unconventional hydrocarbons occurring in economic abundance require greater than industry-standard levels of technology or investment to exploit (Arthur and Cole, 2014). Geological formations that host unconventional oil and gas fields and coal bed methane are extraordinarily heterogeneous and exhibit a wide range of physical and chemical features that can vary over many orders of magnitude in length scale. In the context of subsurface geochemical and mineralogical processes relevant to unconventional hydrocarbon deposits we need to consider both the sedimentological and diagenetic processes that formed the deposits and the present-day nature of fluid and rock properties and the complex interactions among fluids and between solids, fluids and even microbial communities over broad ranges of temperature, pressure, fluid composition, spatial and temporal scales. Of particular importance is nature of the microstructure and evolution of pore space in rocks which are critically important factors controlling multiphase flow.

Many unconventional reservoir lithologies are comprised of pore regimes ranging from relatively uncommon large macropores at the millimeter scale to more numerous small micropores at the sub-micron and nanometer scale (Anovitz and Cole, 2015). The size, distribution and connectivity of these confined geometries, the chemistry of the solid, the chemistry of the fluids and their physical properties collectively dictate how fluids migrate into and through these micro- and nano-environments, wet and ultimately react with the solid surfaces. Our current understanding of the rates and mechanisms of fluid and mass transport and interaction within these multiporosity systems at the molecular scale is far less robust than we would like.

This presentation will take a two-fold approach to this topic area. First we will provide a brief overview on pore types and their relationship with mineralogy in key gas shale formations with special emphasis on the Utica/Pt. Pleasant and Marcellus. We will highlight results from conventional methods such as SEM along with more sophisticated approaches including small- and ultra-small angle neutron scattering that contribute to two key science question areas: (a) What are the size, distribution, connectedness, and contribution to total porosity of nano- to micropores in representative gas shales? and (b) How do these pore features vary with the distributions of clay and carbonate matrix and organic matter?

The second more in-depth part of the presentation will focus the application of state-of-the-art experimental, analytical and computational tools to assess key features of the fluid-matrix interaction relevant to shale settings. The multidisciplinary approaches highlighted will include neutron scattering and NMR experiments, thermodynamic measurements and molecular-level simulations to quantitatively assess molecular properties of pure water, aqueous electrolytes and simple immiscible water-hydrocarbon mixtures confined to well-characterized porous media, subjected to temperatures and pressures relevant to subsurface energy systems (Cole et al., 2013). These studies conducted in concert are beginning to provide a fundamental understanding at the molecular level of how intrinsically different C-O-H fluids behave in confined geometries compared to bulk systems.

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Transport Enhancement of Hydrocarbons in Shale Nanocapillaries: A Multicomponent Study Involving Capillary Wall Effect

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ABSTRACT

The production of hydrocarbons from unconventional reservoirs are of great importance today. A better understanding of this phenomenon lead to more accurate production forecast in petroleum industries. Especially, at new the low oil price era, oil and gas companies are more sensitive to cost and thus eager for reservoir simulation with higher precision to make wiser plans. Unlike flow of fluid in conventional reservoirs, the fluid transport in unconventional reservoirs involves kerogen pore structure with much smaller capillaries. This, in turn, leads to large capillary wall surface area and, consequently, to a significant physical adsorption effect. Measurements are needed to understand the nature of flow inside kerogen structures. However, direct measurements are difficult and have large uncertainties related to kerogen isolation. Non-equilibrium molecular dynamics simulation allow numerical study of fluid transport inside model nano-capillaries representative of kerogen matrices. Now, we have been studying the nanoscale transport of simple hydrocarbons, using carbon nanotubes as the equivalents for kerogen single nano-capillaries. The flow inside the capillary is simulated under various conditions, e.g., capillary diameter, temperature, average pressure, fluid composition and capillary wall morphology, to mimic the actual conditions of unconventional oil and gas reservoirs. Based on the simulation results we observe that fluid flow velocity and mass flux are significant near the capillary surfaces where adsorption takes place. Hence, Hagen-Poiseuille equation based on the no-flow condition at the wall significantly under-estimates the fluid flow in nano-capillary. The dependence of surface transport velocity, as well as flow enhancement, are determined quantitatively. The transport enhancement can be clearly observed using the concept of relative flow rate, or simply by calculating the mass flux across the capillary by multiplying the non-zero surface velocity by the total amount of hydrocarbons across the intersection of the capillary. Transport behavior is additionally controlled by the inner surface morphology, which requires considerable modeling work from the real kerogen structures to fully determine the transport enhancement. Currently, we are expanding the research to more components and their combinations, to arrive at a more precise quantitative correlation for the single capillary system.

Liquid Transport in Nanoporous Media

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ABSTRACT

Darcy flow is the prominent mechanism of fluid transport which is based on the continuum representation of the porous media. However, in nano-scale porous formations, such as those observed in shale reservoirs, transport of fluids exhibit substantially different physics than what is observed in larger-scale systems. Therefore, analysis based on simple Darcy's law yields significantly inaccurate values of permeability and transport of fluids in such nano-scale environments. This leads to an increased need for an accurate description and understanding of fluid transport in the nano-scale structures. In this study, we investigated the nano-scale fluid transport using DI water and 15 to 25 nm diameter SiO2 nano-particles and quantified the boundary velocity slip at the nano-scale medium. Nano-scale fluid transport encounters substantially different physics from continuum descriptions mainly due to the dominant effects of the (i) boundary velocity slip, (ii) surface force field, and (iii) surface adsorption effects. The boundary velocity slip has a great influence on the velocity distributions of fluid flow (1). No slip boundary conditions are assumed in classical fluid dynamics. However, liquid flows in nano-scale confinements exhibit substantial slip for hydrophobic surfaces (2). Further reduction in the pore-size brings more challenges in the effects of the boundary on the overall fluid transport. As the pore sizes in shale reservoir gets down to a few nanometers, water and species transport at such small scales cannot be modeled using continuum fluid dynamics.

We constructed bench-scale flow experiments monitoring the fluid flow using nano-porous medium. We measured the flowrate (Q) over a range of constant pressure conditions, and the measured flow rates are compared to the flow rate predictions based on the pressure driven Poiseuille's equation. The Poiseuille's equation corresponds to the flowrate determination without the influence of the boundary velocity slip or surface adsorption effects (QNS). The boundary effects are determined on the overall fluid transport phenomena by defining the ratio of the flowrates (Q/QNS). Our results have shown that this ratio varied between 1.3 to 2, which indicates that the actual flowrate can be twice of the value determined by the no-slip model. The increase in the observed flowrate is determined to be due to the boundary velocity slip, where the slip length is observed to vary from about 8 to 30 nm for a hydraulic diameter of about 220 nm within the nano-porous media. Such boundary effects can drastically change the fluid transport especially when the slip lengths become comparable to the pore size at the nanoscale confinements and thus need to be incorporated in the fluid transport equations for accurate representation of fluid flow in nano-porous structures. Molecular Dynamics (MD) simulations are also carried out to investigate the breakdown of continuum hypothesis due to scale and wall effects. Using MD simulations we characterized the atomistic behavior of density and velocity distributions (3). Comparing these with the predictions from force-driven Poiseuille flow with constant density and viscosity enables us to detect the variations in apparent liquid viscosity, slip length and density in nano-scale confinements.

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Dynamics of Ultra-Confined Water in Hemimorphite

Presenter: Timothy Prisk
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AUTHORS

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ABSTRACT

Porous media constitute a broad class of natural and synthetic materials that play keys roles in geological processes and the modern chemical industry. The structure, properties, and phase behavior of fluids may be strongly modified from their bulk counterparts when they are adsorbed to solid surfaces or confined within porous media. Water molecules confined within microporous minerals present an extreme example of molecular confinement, where the water molecule is trapped within cages or channels which are not much larger than the water molecule itself. In these materials, individual water molecules or small clusters of water molecules may interact with a highly restricting, anisotropic crystal framework by means of hydrogen bonding.

Hemimorphite is a clear example of a hydrated mineral whose thermodynamic properties and phase behavior are shaped by water molecules and hydroxyl groups under extreme confinement. In this presentation, we report neutron scattering investigations into the structure and dynamics of water confined within hemimorphite and show how they are connected to its properties and phase behavior. The water molecules within the nanocavities of hemimorphite form a two-dimensional hydrogen bond "network" with the framework, in contrast to the bulk fluid where water molecules are tetrahedrally coordinated with their nearest neighbors. The total diffusive motion of the water molecule is a superposition of two processes, one being a slow jumping from one hydrogen-bonded location to another and the other being rapid, localized motions at each hydrogen-bonded location. The first motion is an analog to the rotation of water molecules in the bulk fluid, while the second motion has no known analog in either the bulk or interfacial fluid.

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The effect of geometry on molecular restructuring in nanometer scale pore spaces

Presenter: Ali Qajar
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ABSTRACT

Molecular restructuring inside confined porous media spaces affects the dynamic and thermodynamic properties of the confined fluids (such as their critical temperature and slip coefficient on the boundaries). For instance such phenomenon affects the molecular selectivity in membranes as well as productivity of shale formations. Direct measurements of these physical properties inside nanoporous materials (< 2 nm) is nearly impossible and molecular scale models are a necessity for interpretations of measurements made in nanoconfined media. Simple molecular models usually ignore lateral interactions between the adsorbed molecules and only consider interactions with the pore walls as the dominant ones. Thus they fall short for providing a picture of fluid restructuring inside porous materials. Density functional models and atomistic simulations are considered as more accurate approaches to assess the molecular state inside confined spaces. In our recent works, we have implemented lattice density functional theory (LDFT) model which is an algebraic version of thermodynamic equilibrium models used in conventionally integral DFT models. With LDFT model, we have studied the effect of pore geometry, pore size, surface and lateral interactions on adsorption equilibrium of light gases. The model is derived with dimensionless energy terms, therefore it can be expressed and applied for any real or hypothetical molecule at any given temperature. We have studied how lateral interactions (self-adsorption) between the adsorbate molecules restructures them inside pores at different geometries of slit, cylindrical and spherical pores. The simulations suggest that, for light gases such as CH4 and CO2, near and above room temperature, surface interactions are more dominant than lateral forces. For light molecules only the molecules adsorbed near the surface are compressed into form the ad-layer, while for the heavier molecules such as benzene the restructuring is propagated throughout all adsorbed layers. In addition, for light gases there is much more pronounced shift in the critical temperature of the adsorbed gases than that for the heavier molecules.

THEORETICAL INVESTIGATION OF THE EFFECT OF MEMBRANE PROPERTIES OF NANOPOROUS RESERVOIRS ON THE PHASE BEHAVIOR OF CONFINED LIGHT OIL

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ABSTRACT

Problem Statement, Objectives, Scopes
As hydrocarbons in tight oil reservoirs are primarily stored in nano-sized pores, a particular issue when the sizes of pores and pore throats decrease down to the sizes of hydrocarbon molecules is that nanoporous reservoirs may display membrane properties, acting like a semi-permeable membrane that permits certain molecules to pass through freely yet restricts the transport of other components with larger diameters. This membrane property of nanoporous reservoir will result in compositional differences between different parts of the reservoir and unbalanced pressures even at the equilibrium condition. Therefore, when the membrane effect is present, the phase behavior of reservoir fluids may deviate from the ordinary case, and it is not adequate to use a single composition to characterize the reservoir fluids for the entire nanoporous reservoir. In an attempt to model the effect of membrane filtration can have on production, we developed a filtration model that allows only certain components to achieve chemical potential equilibrium; the restricted components, on the other hand, could not establish chemical potential equilibrium due to size exclusion.
Methods, Models, Procedures
We divided a single-cell nanoporous petroleum system and the multicomponent fluids therein into two parts: one part that is already “filtered” and can flow to a production well without compositional change, and another part that replenishes the “filtered” fluids through a semi-permeable membrane. We modeled a constant-composition expansion process of fluids confined in such composite pore systems using the modified Peng-Robinson EOS equilibrium calculations, assuming that not all of the components can establish chemical potential equilibriums across the membrane. Restriction makes the pressures of the two systems different. The fluid phase behavior and changes in fluid properties such as density, viscosity, bubble point pressure and interfacial tension are calculated and reported at different depletion pressures. By comparing these properties to those computed without membrane, the effect of membrane properties on reservoir fluid properties is illustrated.
Results, Conclusions
We find that membrane filtration makes the produced hydrocarbon mixture lighter, and traps the heavier components in the reservoir, which qualitatively agrees with the expectation. The obtained fluid saturation distributions in the porous medium and the compositions of the produced and trapped fluids, as well as the fluid properties help us better understand the effect of internal filtration may have on the phase behavior and properties of reservoir fluids during a pressure depletion, and may provide us new perspectives to map out potential EOR applications.

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Elastic response of mesoporous silicon to capillary pressures in the pores

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ABSTRACT

When a fluid is adsorbed in a mesopore, it exerts a pressure on the pore walls, which is typically of the order of 10 MPa [1]. This pressure causes deformation of the pore, and as a result deformation of the porous material as a whole. This effect, known as adsorption-induced deformation has been experimentally observed for many mesoporous materials, including mesoporous silicon (pSi). Despite the high pressure, the strains are small so that the deformation is linear elastic, and one can assume a linear relation between the pressure in the pore and the experimentally observed strain with a proportionality constant M, called the pore-load modulus [2]. The knowledge of the pore-load modulus allows to predict the elastic response of a porous material to adsorption, therefore it is useful for application of adsorption-induced deformation to sensing and actuation [3,4].

The pore-load modulus relates the pressure inside the pore to the overall deformation of the sample, rather than relating an external load to a deformation, like Young's or bulk moduli. Therefore an important question is how to relate the pore-load modulus to the material properties of the matrix and the pore geometry. In general, for a material with a wide pore size distribution (PSD) and arbitrary pore morphology and orientation, this question may be complicated. However, for systems such as pSi considered in this work, where the geometry is regular, it can be resolved.

Here we present a dilatometric study of the deformation of a macroscopic pSi membrane induced by adsorption of water vapor. The pSi membrane has parallel channel-like pores. From the experimental strain isotherm we calculate the pore-load modulus. We perform FEM simulations of adsorption-induced deformation of samples with hexagonal and square lattices of cylindrical pores. We find that the pore-load modulus weakly depends on the geometrical arrangement of pores, and can be expressed as a function of porosity. Therefore we relate the deformation of a porous sample to the deformation of a single cylindrical tube from the pressure applied to its inner surface. Based on this model we derive an analytical expression for the pore-load modulus as a function of the porosity and the elastic properties of the non-porous material (Young's modulus and Poisson's ratio). The predictions of our analytical model are in excellent agreement with FEM results. We also achieve good agreement between our experiment and our analytical model for adsorption-induced deformation of pSi, suggesting that the Young's modulus of silicon pore walls could be only slightly lower than the Young's modulus of bulk silicon [5].

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Nanoporous Gold as a Switchable Electrocapillary Pump

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ABSTRACT

Spontaneous imbibition enables the elegant propelling of nano-flows because of the dominance of capillarity at small length scales. The imbibition kinetics are, however, solely determined by the static host geometry, the capillarity, and the fluidity of the imbibed liquid. This makes active control particularly challenging. Here we show for aqueous electrolyte imbibition in nanoporous ?gold that the fluid flow can be reversibly switched on and off through electric potential control of the solid–liquid interfacial tension, that is, we can accelerate the imbibition front, stop it, and have it proceed at will. Simultaneous measurements of the mass flux and the electrical current allow us to document simple scaling laws for the imbibition kinetics, and to explore the charge transport in the metallic nanopores. Our findings demonstrate that the high electric conductivity along with the pathways for fluid/ionic transport render nanoporous ?gold a versatile, accurately controllable electrocapillary pump and flow sensor for minute amounts of liquids with exceptionally low operating voltages.

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Impact of ion adsorption on wettability in oil-water-mineral systems

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ABSTRACT

Wettability alteration is one of the most widely cited microscopic mechanisms to explain the success of low salinity waterflooding in sandstone reservoirs. We performed experiments in highly idealized model systems consisting of oxidized silicon wafers, mica and gibbsite as substrate to mimick the rock, pure alkanes to mimick the oil, and aqueous solutions of various chloride salts of common alkali and earth alkali metals at variable pH to represent the brine. For these idealized systems, we find that water wets mica and silica surfaces for Na+ and K+ ions for all pHs and concentrations investigated. For Ca2+ and Mg2+, however, we find a transition to finite water contact angles of up to 10 degrees beyond a certain threshold concentration and pH [1]. Surface charge measurements using atomic force microscopy along with atomic resolution imaging demostrates that this transition is caused by the strong adsorption of the divalent cations to the solid surface [2]. The result can be explained almost quantitatively in terms of a combined surface speciation and DLVO model. Addition of tiny amounts of polar components fatty acids to the ambient oil increases the maximum contact angle to more than 60 degrees, demostrating the synergistic effect of divalent cations and acidic oil components in setting wettability.

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Mechanistic modeling of low salinity waterflooding processes with cation exchange, mineral dissolution and fines migration 2: numerical solution

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ABSTRACT

The mathematical model for describing oil recovery by low-salinity water injection in core experiments described in a companion work [1] is numerically solved using a finite element method in space and a backward finite difference discretization in time, resulting in full implicit scheme. The model implementation combines some recently published approaches [2] [3], and consists of a set of non-linear coupled PDEs combining oil-water bi-phasic flow with reactive transport associated to cation exchange and mineral dissolution/precipitation and fines attachment/detachment processes. The dynamics of the process is presented for some core flood study cases with different brine salinity. Numerical results for diverse quantities as function of space and time are analyzed and discussed.

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Wettability, brine composition, and waterflood recovery

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ABSTRACT

Over the past 40 years, the working assumption that all oil reservoirs are strongly water wet, and that this is optimum for recovery, has become widely rejected. Wettability, a complex variable that depends on Crude Oil/Brine/Rock (COBR) interactions, has a dominant effect on recovery. Choice of injection brine composition is a practical option for alteration of wettability and related interfacial phenomena during a waterflood. For laboratory floods, variation of connate and/or injection brine composition resulted in differences in recovery of up to 16% PV. In particular, increase in recovery of crude oil with reduced salinity (the Low Salinity Effect, LSE) has been under investigation for over 20 years and over 200 papers on LS flooding have appeared over the past 10 years. Results are divided into LS floods starting at low initial water saturation (LSE@Swi) and at residual oil (LSE@Sor), sometimes referred to as secondary and tertiary mode processes respectively. Extensive data sets show that reservoir rocks, on average, show significantly higher LSE than outcrop. Necessary, but not sufficient, conditions for LS response are the presence of an initial water saturation, crude oil, and clay. Proposed mechanisms include Limited Particle Migration (LPM), saponification, Multicomponent Ion Exchange MIE, double layer expansion, osmosis, interfacial viscosity and the effect of pH on surface electrostatics. None of the proposed mechanisms can predict the magnitude of the improved recovery; most cannot even predict when the low salinity effect will occur. The major obstacle to systematic investigation is the lack of an outcrop rock that exhibits significant and reproducible low salinity effects.
Associated models of LSE range from variation of contact angle in networks of smooth cylindrical tubes, to explain increased recovery by MIE, to detailed analysis of electrostatic interactions at rough surfaces. There is strong interest in application of LS flooding as an enhanced recovery technique because of the comparatively low cost. Field work has progressed from encouraging results for single well and well-to-well pilot tests to full-field implementation.

Investigating of the effect of clay particles on low salinity water injection in sandstone and carbonate reservoirs

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ABSTRACT

Low salinity water flooding as an Enhanced Oil Recovery (EOR) technique refers to the injection of brine with a lower salt content or ionic strength into an oil reservoir. Although the mechanisms have not yet been verified, the solution and surface chemistry as well as rock/fluid interactions have important roles that can be attributed to reservoir minerals being sensitive to small changes in solution properties.
Among the proposed mechanisms, the clay content of rock and type of clay has been of significant interest in shedding light on the low salinity water flooding process. In this paper, three clay types (Illite, Kaolinite and Montmorillonite) have been selected to investigate the individual contribution of each on the rock surface characterization and low salinity water flooding performance for sandstone and carbonate reservoirs.
The results from contact angle measurement on the oil-wet calcite/ sandstone by low salinity water at various temperature show that the presence of low content of illite in the rock materials, in contrast to the kaolinite, reduces the contact angle significantly. The results of the experiment also indicate that samples with kaolinite clay tend to produce higher contact angles than the samples with montmorillonite clay when modified with crude oil. The highest degree of wetting alteration observed for samples injected with the brine having salinity of 2000 ppm. The increase in temperature tends to produce contact angles values lying in the higher end of intermediate-wet range (75o – 115 o) compared to samples treated at lower temperature where the measured contact angle values lying in the lower end of intermediate-wet range.

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Microfluidic Investigation on Interfacial Properties of Crude Oil-Brine Varying Brine Salinity and Composition

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ABSTRACT

Low salinity water-flooding has been identified as an effective Enhanced Oil Recovery (EOR) method, yet the underlying mechanism remains controversial. Extensive studies have been performed on the influence of rock-brine interactions, but very little work has focused upon obtaining a solid understanding of the interactions between oil and brine and how fluid-fluid interfacial properties are influenced by various brine salinity and composition. To examine solution parameter-specific effects upon low salinity EOR, we have developed a microfluidic device for multiphase interfacial testing with length scales comparable to the pore sizes of oil reservoir rock. Microfluidic devices are simple and inexpensive to fabricate and are shown here to serve as a unique platform for high throughput investigations of the low salinity effect. Unlike with conventional core flooding tests,dynamic fluid-fluid phenomena and steady state conditions can be easily visualized within microfluidic devices under a microscope. A microfluidic flow-focusing geometry was utilized to control and observe snap-off of crude oil phases by a shearing brine flow. The size of the generated droplets are examined as a measure of interfacial stability, or the resistance to snap-off. Our results indicate that suppressed snap-off, and therefore a more continuous oil phase, can be observed when the brine with lower ionic strength and monovalent cations is employed. Polar fractions in crude oil, such as asphaltenes are believed to be responsible for the build-up of the interfacial visco-elasticity, which is mediated by the ionic strength and nature of the brine, leading to increased oil phase stability.

Low salinity waterflooding: Mechanisms and applications.

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ABSTRACT

Low salinity waterflooding in sandstone and carbonate reservoirs has been the subject of intensive research for the last fifteen years. The promise of recovering significant amounts of additional oil during normal waterflood operations is an attractive option. The relatively low CAPEX and OPEX means many fields could apply the technique in a profitable fashion, particularly in times of low oil prices. However, while many hypotheses have been advanced to account for the laboratory and field observations, the lack of predictability has limited application of this technique.

The most reasonable proposed mechanism is that of wettability alteration. Current wettability models do not always distinguish between oil directly bound to mineral surfaces and oil that adheres to the mineral surfaces by electrostatic interaction through a water film. However, laboratory and field cases showing incremental recoveries up to 30% of the original oil in place suggests that a large portion of the oil in place is loosely bound to mineral surfaces by electrostatic interaction. This portion of oil adhesion can be manipulated by changing water chemistry and predicted using suitably-modified double layer surface-solute formulations.

The comparison of the current data with predictions from modified geochemical models is illuminating. The results of the models show that most of the field and laboratory observations including changes in pH, effluent water chemistry and incremental oil production can be explained as water-oil-rock reactions. Using this basis a quantitative screening tool was developed to identify fields with high probabilities for favorable outcomes.

A range of fields judged favorable were then evaluated for potential profitability using public-domain data and an analog model based on the Kinder Morgan CO2 scoping tool. While we did not include peripheral benefits such as lower maintenance costs, reduced scaling and souring and improvement in injectivity, it is evident that low salinity waterflooding can be very profitable for many fields. In cases where water treatment of produced water before re-injection is required, costs are modest assuming reverse osmosis technology. Other cases where target injection chemistry can be achieved by blending produced water with other resources are even more profitable.

Revisiting the mechanisms of clay damage

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ABSTRACT

Over the last years, numerous authors have noticed that oil recovery can be enhanced by manipulating the ionic content of injection water. The ions to be used depend principally on the type of formation in which the water is being injected. However, the underlying mechanisms that lead to an increase in oil recovery are still not clear. The interactions between fluids-ions-rocks are not well understood.

In the particular case of clays minerals, they are encountered in all type of formations. Under interaction with water, clays undergo two phenomena that have a major and direct impact in permeability impairment: (1) swelling effects, and (2) instability of the structure. The former has been widely studied and rather well characterized, but the latter is still to be explained properly. Since the decade of the 70's, some authors hypothesized the means by which ions and clays interact, becoming the conventional wisdom over all related processes are based on, low salinity waterflooding being among them. During the last few years, molecular dynamics (MD) simulations opened a door to explore such phenomena at molecular scale, providing microscopic pictures that allow us to gain new understanding, reinterpret what is commonly accepted, and propose new explanations.

In this work, we carried out MD simulations to review the mechanisms of clay damage under hydration, the manners clays interact with water and cations, the structures they form in between of aluminosilicate-sheets, and offered an alternative explanation to how clay structures become instable after certain water concentration. Water molecules form one, two, and sometimes three layers parallel to the surface of clays. The cations already present in montmorillonites (the most representative of the smectites) or coming with low salinity water will either be adsorbed by the clay surfaces or become fully hydrated, detached from the surfaces and located in the midst of the interlayer space between clay surfaces, while water molecules that do not hydrate the cations invade the clay structures, making them unstable. The driving force of this phenomenon happens to be the hydration energy of the cations in question.

Transport and deposition of solid particle in porous media: experimentation and modelling

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ABSTRACT

Damage and plugging of the granular structure of oil reservoirs are commonly observed during the the process of Produced Water Re-Injection (PWRI). The produced water contains usually solid particles and oil droplets which can deposit in the pores of the medium and lead to a significant decrease of the reservoir permeability around the injectors and affect the injectivity of these wells. In this work an experimental study on the transport and deposition of silica particles in a dense sand sample subjected to flow is presented. A semi-analytical model is also developed, which permits to simulate the injection pressure evolution during the PWRI process. The experimental study is performed on an injection cell in which a cylindrical sand specimen (height 80 mm, diameter 80 mm) is put under isotropic stress. Water containing a low concentration of fine particles (diameter of few microns) is injected at a constant flow rate. The evolutions of the sample mass and of the injection pressure are recorded. The experimental results show an increase of particles mass retained inside the sample during the injection and an increase of the injection pressure attributed to a decrease of the permeability of the sample. They also show that despite the low concentration of particles of the injected fluid, a clogged area of a few centimetres (generally called a cake) forms at the flow inlet. The analysis of this area by mercury porosimetry showed a significant decrease of the porosity and of the pore size and the formation of a new family of pores formed by the agglomerated particles (Feia et al. 2015).
A semi-analytical model is proposed for describing the effect of particles deposition on the evolution of the pore pressure at the inlet of the injection. A mathematical function for the spatial distribution of the deposited particles is assumed and a double porosity medium is considered in order to account for the porosity of the internal cake. The evolution of the permeability with the evolving porosity is described by a power law. The model can accurately simulate the pore pressure evolution during the fluid injection experiments.

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Mechanistic modeling of low salinity waterflooding processes with cation cation exchange, mineral dissolution and fines migration 1: theoretical model

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ABSTRACT

A mathematical model has been derived to describe some of the main mechanisms mentioned in the public literature as most relevant for oil recovery by low salinity waterflooding at laboratory scale. The model is based on some previous models [1] [2], and specifically considers cation exchange, mineral dissolution/precipitation reactions, as well as fines release, migration and flow path clogging. The effect of the salinity reduction on the relative permeability and capillary pressure curves are introduced as parametric changes in standard models. The change in absolute permeability due to salinity reduction is related to the release and clogging of fines. A coupled PDE system for the two-phase flow, chemical species transport, and fine dynamics has been established for conditions resembling core waterflooding experiments. The numerical solution and results analysis are presented in a companion work [3].

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Impact of salinity on the pore scale distribution of crude oil in rock

Presenter: Maja Ruecker
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ABSTRACT

Flow behavior and displacement efficiency during immiscible displacement in porous rock is significantly influenced by the wetting state of the fluid-rock system. This has a large impact on many multiphase flow problems, for instance during oil recovery. During various field studies [1,2] it has been shown that by lowering the salinity of injected water, the recovery of crude oil can be improved, both in sandstone and in carbonate rock, which is the so-called low salinity effect. Although the method was proven in various field studies [1,2], the processes leading to the increase in production at the Darcy scale are still not fully understood at the pore scale. Most studies published in literature agree that the application of low salinity brine leads to an effective wettability change in the rock. This view is supported by models [3] and also by X-ray computed micro-tomography (µCT) which allows visualization of the initial and end-state of a low salinity experiment [4]. But so far it has not been possible to directly observe how the wettability change leads to the incremental production of oil during a low salinity flood. In this study we directly observe the effect of varying brine compositions in real time in 3D in sandstone and carbonate rock by using synchrotron beamline-based fast X-ray computed tomography.

The micro-CT flow experiments with low salinity brine were conducted in tertiary mode, i.e. by first performing a high salinity water flood followed by a low salinity waterflood, which were both imaged in-situ in real-time at 3s scanning time. The 20mm long and 4mm wide rock samples were prepared in advance by saturating them first with high salinity brine and then with crude. In order to establish reservoir conditions, the rock the samples were “aged” by applying 30 bar pressure and 70C temperature for one week. The high salinity brine contained 200g/l potassium iodide (KI) and the low

salinity brine 27 g/l KI. KI was chosen due to its qualities as contrast agent. Therefore not just the change of the oil phase configuration could be observed but also the dispersion of the low salinity brine in the high salinity brine.

The images give first insights into how and where in the rock low salinity affects the flow behavior during forced imbibition. The results show the mobilization of the oil phase. Beside connection and disconnection of the oil phase through thin pore throats as observed before in imbibition [6], these experiments clearly show a movement of the oil from pore throats to pore bodies at the transition from high salinity brine to low salinity brine for sandstone and carbonate rock.

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Asymptotic modelling of jump conditions at a fluid-porous interface

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ABSTRACT

This work proposes an asymptotic modelling \citep{A03} 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 transition region $\Om_{fp}$ 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 $\Si$ separating the homogeneous fluid and porous regions. These interface conditions for the jumps across $\Si$ 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.
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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 \citep{BJ67,OTW95a,VAOTG13} 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 equation for the pressure jump which does not vanish {\em a priori} as soon as there is a non-zero transverse flow at the interface.

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Numerical investigation of the interface between porous media and a transpiration-cooled turbulent channel ?ow

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ABSTRACT

Transpiration cooling is an active cooling technique able to reduce thermal loads of applications exposed to extreme operation conditions such as rocket thrust chambers. Since passive cooling techniques, e.g. radiation cooling, are limited and nonadjustable during ?ight, transpiration cooling might offer a promising alternative. The basic idea of transpiration cooling is to inject a coolant through a porous material into the hot gas ?ow boundary layer such that the temperature boundary layer thickens and a coolant ?lm develops. This leads to a signi?cant reduction of
the heat load at the wall. The coolant is driven through the porous material by a pressure difference between the coolant reservoir and the hot gas ?ow.
The present study numerically investigates the in?uence of the cooling gas injection on the temperature, the velocity and the local skin friction in the boundary
layer of a subsonic turbulent hot gas channel ?ow. Here, the hot gas in the channel ?ows over a cooled porous ceramic matrix composite (CMC) material. Separate solvers are used for the hot gas ?ow described by the compressible Reynolds-averaged Navier-Stokes equations and for the porous medium ?ow of Darcy-Forchheimer type. The two solvers are directly coupled with each other through alternating data exchange at the interface. Since the goal is to achieve a steady state solution, the coupling is realized in a weak sense, i.e., both solvers are applied alternately and converged to a steady state with respect to the coupling conditions generated from the solution of the other solver at the particular step of the iteration process [1]. Therefore the coupling conditions are a crucial part of the model. The numerical methods developed and implemented for the solution of the coupled problem are described in detail in [2].
Simulations are based on a con?guration for which experimental data are available from Schweikert et al. [3]. The test case at hand is performed for an in?ow Mach number of M = 0.3 and an in?ow temperature of T = 425 K. The numerical results are compared with the experimental data to validate the two solvers as well as the coupling and to provide complementary insight into the effects of the cooling which cannot be easily assessed from experimental measurements.

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Development of A Unified Solver for Coupled Fluid, Porous, and Material Response Problems

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ABSTRACT

In hypersonic planetary entry missions, charring ablative material is often used as the heat shield material in Thermal Protection System (TPS). This kind of material is usually made of a porous matrix (such as carbon fibers), and impregnated with resins. It is designed to resist the severe aerodynamic heating by dissipating part of the energy through ablation (the process of solid mass loss due to heating), and pyrolysis (usually endothermic). Due to the increasing challenge of recent and future space exploration missions, most of the existing charring ablative solvers are experiencing two major difficulties: 1) lack of models and/or dimensions to capture certain phenomena; 2) troublesome interface coupling between fluid field and porous material.In order to overcome these obstacles, the authors developed a versatile 3D char- ring ablative solver, named as Kentucky Aerodynamics and Thermo-response System (KATS) - Unified Solver (US). The solver is based on finite volume method, featuring second order spatial and first order temporal accuracy. It also utilizes techniques of domain decomposition to parallelize the computation. The greatest advantage of a unified solver is that, the fluid dynamic solver and the material response solver are coupled seamless. For instance, there is no need to track the material recession surface, which is tedious using the current state-of-the-art methodology. In addition, unifying the solvers makes it possible to model the gas surface interface reaction in the boundary layer with high-fidelity models.In this work, the governing equations and the numerical framework are largely derived from the authors' previous work [1]. However, the material properties are handled differently to account for the change of matter in different regions. For example, in the plain flow region, the material porosity is set to be one, and the permeability is set to be 1E10 times of the value in the porous region. This enables the computer code to solve the Navier-Stokes equations in the flow field using the same set of governing equations. The solid decomposition rates, which were solely used in the material response solver, are also set to zero for the plain flow region.
At this initial stage, the development of KATS-US shows some promising results, via code-to-code verification with several published test cases. Specifically, the Beavers- Joseph flow problem and a porous plug problem are simulated and compared with Costa et. al. [2] and Betchen et. al. [3]. The results of these two problems are presented in the attached figures. These results clearly demonstrate that KATS-US is capable of solving coupled plain and porous flow problems. Moreover, the difficulty in assigning boundary conditions (especially the ones touching two regions) can be circumvented by assigning an extra length of geometry, as depicted in the Beavers-Joseph problem test case. The next step of this work is to model the chemistry of material ablation (oxidation) and the transport of pyrolyzing species.

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Liquid Water Transport between Gas Diffusion Layer and Gas Channel in a Polymer Electrolyte Fuel Cell

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ABSTRACT

Understanding water transport between the gas diffusion layer (GDL) and the gas channel (GC) is crucial to the water management of PEFCs. Numerically, it is challenging to model the coupled two-phase flow between porous media and free flow (i.e. mini GCs).
This talk includes two parts. Frist, a macro-scale model for liquid water flooding in the GC is presented. It is phenomenologically developed based on several assumptions. It is used to illustrate water flooding and gas pressure loss in the GC under different operating conditions.
In the second part, a pore-scale dynamic network model for water flooding in the GDL and GC is presented. An assumed network structure is used to represent a mini GC, which is coupled with the pore network of the GDL with a proper interface configuration. The pore-scale results are used to verify macro-scale models. Also, constitutive relationships can be provided.

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Dragforces on Particles at Heterogeneous Interfaces between Porous and Free Flow Domains

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ABSTRACT

Free fluid flow adjacent to a permeable porous layer is a well known and often discussed transport problem. One application in this context is sediment erosion and deposition of solid particles. Therefore different approaches to model the evaluation of sediment transport and appropriate initiation of motion of solid particles exist, e.g. models for a Darcy-Brinkman approach provided by Neale and Nader [1], a two-domain approach by Beavers-Joseph [2] and an one-domain formulation by Ochoa-Tapia-Whitaker [3]. These approaches present total or partial domain approximations for the bed shear stresses or the corresponding shear velocity at the interfacial transition zone that separates a free Stokes-flow domain and a porous Darcy-flow domain. Based on these approximations the models define critical states for which sediment transport or even motion of single solid particles is initiated. These macroscopic approaches present approximated values for critical shear stresses or critical shear velocities, most commonly only based on the occurring flow velocities. However, as indicated, for that these approaches do not take the microstructure heterogeneity in the transition zone into account. To overcome this limitation we present pore-scale resolved direct numerical simulations (DNS) to analyze the velocities and shear stresses as well as drag and lift forces on solid particles in the transition zone. We use a weakly compressible Smoothed Particle Hydrodynamics (SPH) scheme [4,5] to simulate single-phase fluid flow.
SPH as particle method of Lagrangian character presents a good choice to model this particular non-linear problem. We implement a two dimensional initial boundary value problem with a heterogeneous microstructure with nearly closest packing of solid grains at the lower part of the domain and a free flow region of the same size on the upper part of the domain where finally parallel flow driven by volumetric forces is applied.
Our simulations allow a comparison between the effective velocity and shear stress profiles and the previous presented analytical models to critically assess their validity [6]. Moreover we evaluate the occurring drag and lift forces and thus the influence of the heterogeneity of the interface by introducing different microstructures with varying heterogeneities on the interface. Future work includes the effective analysis of distinctive parameters for the initiation of motion of single solid particles. The resulting information on forces on solid particles can be used for further investigations and simulations of thin suspensions.

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Coupling of Mass, Momentum and Energy at the Interface between Free Flow and Porous Media Flow

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ABSTRACT

Coupled systems of free flow and flow in porous media appear in a wide range of industrial and environmental processes. Basically, two kinds of approaches have been developed for modelling such systems: In the single domain approach, both regions of free flow and porous media flow are regarded as one single domain where one single equation, e.g. the Brinkman equation (Brinkman, 1947), is solved. The interface is accounted for by a variation of spatial parameters. The second approach involves the use of a sharp interface between the free flow and the porous medium which couples both regions where different sets of equations hold, i.e. the (Navier-) Stokes equations in the free flow and Darcy's law in the porous medium. Commonly, this interface devoid of thermodynamic properties ensures the continuity of fluxes as well as thermodynamic equilibrium at the interface between the two domains (e.g. Mosthaf et al., 2011).

However, this sharp and “simple” interface does not allow to resolve potentially import interface processes such as evaporation in detail as it only considers averaged quantities. To tackle this issue, a novel approach is developed where the interface region is described by a dynamic two-phase pore network model which couples the free flow region with the porous medium. This results in a model comprising three domains: the porous medium described by Darcy'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. Mathematically and numerically it is foreseen to couple these three domains using mortar elements (Mehmani and Balhoff, 2014).

As a first step, a dynamic two phase pore network model using a fully implicit Euler time discretization scheme is developed which facilitates the integration of the resulting non-linear system of equations into a global matrix which also includes the systems of equations of the porous medium and the free flow domain, as well as coupling conditions. This model is validated against an established pore network model (Joekar-Niasar et al., 2010) which relies on an IMPES (Implicit Pressure, Explicit Saturation) scheme.
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 modelling evaporation processes.

Furthermore, a two-phase coupling approach is developed which ensures the continuity of mass, momentum and energy fluxes at the model domain interfaces.

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Modeling Buoyancy-Driven Flow in Underground Mine for Geothermal Energy Recovery

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ABSTRACT

The concept of recovering geothermal energy from abandoned underground mines via mine water has been attracting impetus all over the world in recent years. The hypothesis is that mine water accesses to the Earth heat through factures and fissures in the surrounding geologic formations and consequently, the system of mine water and surrounding geologic formations can be used as a higher-grade geothermal reservoir. Field observations has proven that water in closed mines contains a great reserve of geothermal energy (10-50), such as in Poland [1], Netherlands [2], Germany [3], and Spain [4]. However, the scientific understanding of this application is still in a preliminary stage, leading to a limited number of detailed numerical simulations involving both hydrodynamics and physical process in porous materials. The study was therefore conducted to pioneer modeling the buoyancy-driven flow in an underground mine coupled with heat transfer between the mine water and the surrounding porous geologic formations with a representative real case in Upper Peninsula in Michigan. The in-situ measured data were used to validate the developed model. Discusses were also made to provide a better understanding of mechanisms of hydrodynamics in mine water for further geothermal applications.

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Modeling drying in paper-like thin porous media after coupling slow-drying inside with outside flow

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ABSTRACT

The talk will present a fully-coupled method to solve the isothermal slow-drying of porous media after accounting for its interactions with the outside laminar flow from top and bottom sides. The invasion-percolation algorithm will be used to simulate the capillary force driven liquid-flow in the pore-network representing the porous medium. The model based on the pore network accounts for advective mass flux in the external flow field, diffusive vapor-flux in both the external field and internal pore network, the crucial coupling of mass-flux at the porous medium-open channel interface, as well as the film effect inside the porous medium. The validation and accuracy of the proposed method will be discussed. The overall drying rate as a function of time as well as development of saturation distribution with time will be studied as a function the porous-media micro structure.

Multi-scale dynamics of transport in Li ion batteries and limitations of macroscopic Models

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ABSTRACT

Batteries are electrochemical energy storage devices that exhibit physico-chemical heterogeneity on a continuity of scales. As such, battery systems are amenable to mathematical descriptions on a multiplicity of scales that range from atomic to continuum. The need for predicting the system behavior under time dependent forcing over large spatial (system level) and ultra-long time scales (thousand of cycles) requires the adoption of spatially and temporally averaged (continuum) equations. Model accuracy is critical when predictions are needed to accurately estimate macroscopic battery response, including battery lifecycle, SoC and SoH. Macroscopic models treat the electrode as a continuum and are often employed to describe the mass and charge transfer of lithium since they are computational tractable and practical to model the system at the cell scale. Yet, they rely on a number of simplifications and assumptions that may be violated under given operating conditions. Based on perturbation methods of pore-scale equations, we derive the applicability conditions of macroscopic models in terms of relevant dimensionless numbers. Such conditions can be adaptively employed to establish when an algorithm refinement is necessary in order to preserve model predictivity and accuracy. Finally, we discuss how the new proposed tool can be used to assess the validity of macroscopic models across different battery chemistry and conditions of operation.

Macroscopic Electrochemical Properties from Local Microstructural Data

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ABSTRACT

A theoretical framework is formulated to analytically quantify the effects of the microstructure on the average properties of porous electrodes, including reactive area density and the through-thickness tortuosity as quantified (analytically or numerically) from experimentally-determined tomographic sections. The proposed formulation includes the microstructural non-idealities but also captures the well-known perfectly spherical limit. The effects of particle alignment, through-thickness non-idealities, size distribution. etc., on the Bruggeman exponent are quantified as the aspect ratio varies from needle- (or prolate) to or fiber-like (or oblate) shapes. Similarly, the effect of microstructure on electrode reactivity density is quantified. Microstructural conditions where tortuosity can be dramatically suppressed and reactivity maximized are highlighted and discussed.

Multi-scale, multi-dimensional electrochemical transport in porous electrodes for energy storage and desalination

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ABSTRACT

Rechargeable batteries are potential solutions for energy storage on electric vehicles and the electric Grid. In these devices, the electronic charge delivered to an external circuit (as well as the efficiency with which it is delivered) depends on the internal resistance due to the transport of ions and electrons. These transport processes are coupled through electrochemical reactions with electroactive materials that store charge inside porous, composite electrodes. These electrodes contain a heterogeneous distribution of materials (electron conductor, electrolyte, and electroactive material) that facilitates the simultaneous transport and storage of charge. Multi-scale porous-electrode structures can produce enhancement in the capacity and efficiency with which such cells operate. Here, we utilize computational models of granular mechanics and electrochemical transport to optimize nano- and micro-structures of Li-ion battery electrodes. For thin, high-power electrodes we show that columnar order developed by packing of non-spherical LiFePO4 platelets inhibits the solid-state transport of Li ions, but this effect can be mitigated by mixing with inactive, equiaxed nanoparticles that prevent deleterious ordering [1]. For thick, moderate-power electrodes we predict that electrolytic ion-transport is enhanced in composite, graphite-platelet electrodes that are structured with tortuosity at two disparate microscopic scales [2]. We also introduce a novel electrochemical device used to desalinate water whose design was developed using two-dimensional, flowing porous-electrode theory [3].

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Characterizing Porosity and Defect Evolution in Commercial Li-Ion Batteries

Presenter: Jeff Gelb
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ABSTRACT

With the growing global reliance on energy storage solutions for transportation, grid-scale storage, and personal electronic devices, Li-ion batteries are presently at the forefront of modern research. Owing to the high volumetric and gravimetric energy densities, Li-ion batteries are well suited to address many consumer demands, ranging across many different scales and applications. At their core, Li-ion batteries are supported by porous electrodes, facilitating electrochemical activity via ionic transport mechanisms. While this design is widely used, the precise natures of the electrode structures remain poorly understood. Furthermore, the mechanisms for both functionality and failure of the batteries are not well characterized, with short circuits and venting occasionally occurring on packaged, qualified products.

In our research, we have used multi-length scale microscopic investigation to characterize a commercial 18650 Li-ion battery from the pack to the pore scale. 3D X-ray microscopy (XRM) was initially used to survey the battery, producing a 3D volumetric representation of its internal structure without opening the package. The cell was subsequently depackaged and imaged using correlative high-resolution FE-SEM and light microscopy, revealing the multi-scale nature of the cell and particle/pore networks. Individual sections of anode, cathode, and separator were then isolated for 3D analysis using nano-scale XRM. The results demonstrated the power of 3D visualization for battery inspection, and ultimately produced a series of pore-scale models suitable for transport simulation studies. This provided a unique insight into the battery's performance characteristics, supporting the electrochemical analysis with actual microstructure input.
In the second phase of our study, a second battery from the same manufacturer was imaged in its pristine state using XRM, cycled 100 times, and then imaged again. The XRM approach provided the unique ability to observe the evolution of battery mesostructure as a function of cycling on the same cell, in a so-called "4D" investigation. The results showed cracks forming in regions of high tensile stress, which may ultimately help to explain some aspects of the reduction in batter capacity as a function of aging.

Within this series of experiments, we are actively building a research framework for future characterization studies on battery materials. Using microstructural imaging in tandem with electrochemical analysis, a more complete description of the battery materials may be realized. The results from these characterizations provide valuable insight into how batteries perform, evolve, and, ultimately, fail.

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Mesoscale Modeling of the Physicochemical Interplay in the Li-Sulfur Battery Porous Cathode

Presenter: Partha Mukherjee
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ABSTRACT

Lithium-sulfur (Li-S) batteries are a promising energy storage technology, especially in the context of beyond-lithium-ion battery chemistry. However, the Li-S battery still faces several challenges. The transport of intermediate discharge product species between the cathode and anode (“shuttle effect”) causes active material loss, and leads to capacity fade. The precipitation of insoluble discharge products, especially Li2S, alters the cathode microstructure and may adversely affect long-range and short-range transport characteristics. The cathode microstructural change may also cause mechanical stress. Therefore, it is critical to understand the underlying physicochemical interplay due to the microstructural evolution in the porous cathode of the Li-S battery. In this work, a mesoscale modeling approach, which combines microstructure-level transport and interface interactions, will be presented.

Nonequilibrium Thermodynamics of Porous Electrodes

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ABSTRACT

Li-ion batteries often involve electrode materials, such as iron phosphate and graphite, which separate into Li-rich and Li-poor phases upon intercalation of lithium. Classical porous electrode theory focuses on diffusion in the electrolyte and host solid, coupled by Faradaic reactions, but does not describe the thermodynamics of the active material, resorting instead to fitting the (equilibrium) open circuit voltage. This talk describes a reformulation of porous electrode theory based on nonequilibrium thermodynamics, which unifies and extends the Cahn-Hilliard and Allen-Cahn equations for chemical kinetics and charge transfer [1-3]. The reaction rate depends on concentration gradients, elastic coherency strain, and other thermodynamic non-idealities. The theory predicts some surprising dynamical phenomena, such as suppression of phase separation in nanoparticles and mosaic instability in porous electrodes, which have since been observed experimentally, not only for Li-ion batteries, but also for other chemical systems.

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A Finite Element Based Cahn-Hilliard Model for LiFePO4 Battery Cells

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ABSTRACT

Lithium iron phosphate (LiFePO4) is a promising material for rechargeable lithium ion batteries due to its inexpensiveness, safety and long life. These virtues of LiFePO4 as a cathode material have prompted many studies to investigate coating and doping in order to improve the cell's performance. However, in many cases these studies have not fully explained the effects on lithium ion diffusion and phase transformation due to the intrinsic difficulty and complexity of the transport processes. Several lithium intercalation compounds including LiFePO4 exhibit phase separation and the Cahn-Hilliard phase field theory (CH) is central to the study of the resulting coupled electrochemical phase equilibrium transport phenomenon [1]. The Cahn-Hilliard equation (CHE) is characterized by fourth-order spatial derivatives, so casting it directly in its weak form results in the presence of second-order spatial derivatives, and the resulting problem cannot be solved using standard Lagrange finite element basis functions.

This difficulty is overcome in this work by using the COMSOL Multiphysics® software and its Weak Form PDE interface to recast the CH as a system or two coupled second-order differential equations in concentration and chemical potential. Lithium ion battery current and voltage responses enter the model via Butler-Volmer kinetics and the model is verified by reproducing established literature sources for a typical 100 nm LiFePO4 particle. The auxiliary continuation parameter sweep capability in the COMSOL software was especially important for modeling the steep gradients associated with spinodal decomposition of LiFEPO4 into multiple phases for enthalpy of mixing per site above approximately 8.0 J. Figure 1 shows the filling fraction of surface sites during 0.5 A/m^2 intercalation as a function of dimensionless time for enthalpy of mixing ranging from -8.0 to 8.64 J.

The abrupt decomposition into a lithium rich phase near the particle surface and a lithium poor phase in the particle interior is clearly depicted at about 20 dimensionless time units. Figure 2 shows that the characteristic voltage plateauing of the LIFePO4 cell occurs for increasing enthalpy well before phase transformation is initiated. Figure 3 demonstrate an interesting phenomenon for a mixing enthalpy of 8.64 J where the particle initially undergoes single phase filling up to a filling fraction of about 0.3, dual phase filling for filling fraction 0.3 to 0.7 and single phase filling again above filling fraction of 0.7.

Reduced order models for online lithium-ion battery management systems

Presenter: Matteo Icardi
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ABSTRACT

Online battery management systems in hybrid and electric vehicles are an important element to optimise and improve batteries reliability and driving performances. They are typically based on simple ordinary differential models (i.e., equivalent circuit models), calibrated against a huge amount of experimental data. The collection of charge and discharge current to voltage curves has to be performed separately for many different operating conditions (e.g., temperature, state of charge) and is therefore very expensive and time consuming. This fitting procedure is often affected by instability and sensitivity with respect to operating parameters and experimental data. Furthermore, the calibrated parameters do not have any direct physical meaning and the choice of the numbers of parameters (i.e. the order of the model) has to be done on a case by case basis.
We propose some mathematical techniques to derive new robust low-order differential models, starting from the system of partial differential equations of the porous electrode theory (i.e., Newman-type models). This approach allows to define physically-based effective parameters and functional dependences between them. The key point behind this approach is the consideration that a full description of the battery is often not needed and the relation between global quantities of interest might present relatively simple dynamics for most of the battery operating conditions. The main assumptions and limitations behind the Newman's model and its reduced order version are highlighted and a multiscale approach to overcome some of them is proposed.

Processing-Performance Correlations in Porous Rechargeable Batteries

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ABSTRACT

The links between processing, microstructure, and electrochemical properties in rechargeable batteries are often overlooked in the manufacturing of porous energy storage devices, even though the identification of these correlations are key to the development of advanced portable storage technology, particularly for high power density applications. Specifically, the selection of rolling, compaction, and calendaring conditions, all define the instantaneous macroscopic energy density, and are constrained by the starting powders, its morphology and size distribution. Key quantities such as tortuosity, reactivity, and microstructural inhomogeneities are a direct result of this selection plus fabrication process, but are only included by simple trial and error approaches.

In this context, by using as input mechanically stable microstructures generated through an enthalpy-based granular mechanics modeling approach, we are directly exploring the impact of processing on the microstructural polarization losses in porous rechargeable battery electrodes by systematically exploring fundamental, non-spherical particle shapes, in the limit of very low porosities. Topologies and battery architectures that are optimal for battery performance are identified and summarized into graphical representations that enable manufacturers to make a cost-effective selection.

Modified electrospun carbon nanofibers for electrochemical applications

Presenter: Daewoo Han
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ABSTRACT

Electrospinning is the most versatile technique to produce nanofibrous membranes because of (a) straightforward and cost effective setup; (b) controllability of nanofiber diameter from μm to nm range; (c) multitude of electrospinnable materials. Electrospun nanofiber membranes have an extremely high surface area with highly porous structure. This versatility can be further expanded by coaxial/triaxial electrospinning which can produce the multi-layer structured fibers in a single step.1-3 Multi-layer structured nanofibers provide the freedom of novel material development which enables: (1) combination of two different properties from each layer into a single fiber; (2) encapsulation of functional materials (e.g. drug molecules) into the fiber core and its controlled release; (3) electrospinning of normally non-electrospinnable materials, etc.

We have utilized the modified PAN-based carbon nanofiber membrane for sensor applications.4 PAN-based CNF was fabricated by carbonizing electrospun PAN fibers at elevated temperature and it has been utilized to modify glassy carbon (GC) as a new electrode material for the simultaneous determination of trace levels of heavy metal ions such as Pb2+ and Cd2+ by anodic stripping voltammetry (ASV). Due to its high surface area, high porosity and hydrophilicity, we have obtained the 8-fold higher detection sensitivity for lead using the CNF/Nafion modified GC electrode compared to that of a bare GC electrode, as shown in Fig. 1. Low detection limits of 0.9 and 1.5 nM have been obtained for Pb2+ and Cd2+, respectively. These values are well below the allowable limits in drinking water instituted by the World Health Organization (WHO).

Highly concentrated gold nanoparticles have also been successfully incorporated into the carbon nanofiber membrane (Fig. 2) to improve the electrical conductivity and electrochemical performance. Potentially, incorporated gold nanoparticles also provides the selective detection of sulphur- /thiol-based molecules in electrochemical sensor applications.

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Why quasi-static approaches cannot be used to model imbibition relative permeability

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ABSTRACT

Pore scale modelling pioneered by the work of Geoffey Mason [1] has given rise to industry wide activities in the domain of Digital Rock. One of the most common applications for Digital Rock is the prediction of relative permeability. Much progress has been made since in terms of the applied methodology. Currently one of questions is whether quasi-static approaches (like quasi-static pore network modelling) are describing the pore scale displacement physics sufficiently well for this purpose, or whether computationally much more costly dynamic approaches are required. Dynamic approaches that explicitly model the movement of liquid-liquid interfaces cover viscous and capillary forces simultaneously and capture naturally a wide range of pore scale displacement phenomena. But are they really absolutely required to model relative permeability or rather a “nice to have” that capture effects which are in the end not that relevant ?
A comparative study between a quasi-static pore scale modelling approach conducted directly on the pore space of rock and 3D fluid distributions obtained from a 2-phase flow experiment under dynamic conditions imaged with synchrotron beamline-based fast X-ray computed tomography [2] is now able to answer this question with a clear “yes” at least for imbibition.
The comparison shows good agreement between connected pathway flow simulations conducted directly on the 3D fluid distribution obtained from the synchrotron beamline experiment on Gildehauser sandstone rock [3] with a conventional “special core analysis” steady-state relative permeability measurement on a twin-sample. A quasi-static morphological approach to model pore scale fluid distributions, however, shows large discrepancies with the experimental data. The issue with quasi-static methods is not so much the modelling of the Navier-Stokes flow, but rather the description of the pore scale fluid configurations resulting from immiscible displacement events. Direct imaging of pore scale flow experiments by tomography [2,3] clearly shows that pore scale displacement events are cooperative, non-local processes involving many pores which is conceptually different than simple percolation models and quasi-static pore network models predict.
In particular in imbibition we find a complex interaction between film swelling and corner film flow and the breakup of clusters. When following the transition from a connected phase flow to individual

clusters, at the onset of oil mobilization which occurs at relatively large oil saturation, the main mechanism is snap-off leading to a breakup of clusters. The large meniscus oscillations initiated by the snap-off, on the other hand, also leads to coalescence events, which again points to the cooperative dynamics in the ganglion dynamics regime [3]. These cooperative, non-local displacement events are not captured by quasi-static modeling approaches which operate entirely in the capillary regime. Respective pore scale fluid distributions are significantly different from experimental measurements. As a consequence also the respective relative permeability is significantly different than those observed in the experiment.
Therefore, ultimately only dynamic approaches are really able to correctly describe the pore scale displacements and respective pore-scale fluid configurations which are imperative for the correct description of phase connectivity, fluxes of connected and disconnected phases and ultimately relative permeability.

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Disorder is Not Random: The Structure-Property Relationship in Granular Porous Media

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ABSTRACT

Of Geoff Mason's many insights, the most extraordinary was his recognition that Finney's physical model of a simple liquid could also serve as a model porous medium. The crucial element was Finney's painstaking quantification of the spatial coordinates of each sphere in a large, dense, disordered packing. Mason realized these data could be used to identify unambiguously both pore bodies and pore throats in this porous medium. This realization set the stage for completely and exhaustively quantifying the geometry and topology of the pore network, the first time this had ever been done for a nontrivial porous material – and the only such characterization subsequently available for several decades. Analysis using Mason's approach has yielded a rich set of insights regarding the relationship between pore structure and macroscopic properties of granular material. One highlight is the counterintuitive finding that the geometry of pore space is not random. Instead pore dimensions are spatially correlated, and the correlation quantitatively alters macroscopic properties and fluid displacements. Standar theories neglect this correlation and thus leave out an essential feature of this class of materials. The influence of spatial correlation increases as the connectivity of pore space becomes poorer, making these considerations relevant to the current focus on the sedimentary rocks in shale gas and tight oil reservoirs.

Capillary Driven Imbibition onto Pores of Precisely Controlled Geometry

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ABSTRACT

In an attempt to find out how the viscosity ratio of the two fluids affected imbibition, Prof Morrow's group used a range of mineral oils to displace air from an initially dry Berea sandstone core. This was instead of the usual brine/oil combination. The results were unexpected. The oils imbibed ten times faster when the displacement was co-current than when the displacement was counter-current. Ten times is a very significant difference. So why is it? One explanation is that the imbibing oil reduces the relative permeability to air at the active face by a factor of ten. But this is unlikely to be the rate-determining factor. Others also think this unlikely too because, in the continuum theory for water-air displacements, the mobility of the non-wetting phase (air) is usually assumed to be infinite. Another explanation is that the pressure required to blow the air out of the core as bubbles is quite close to the capillary pressure generated by the pores in the rock. But this back pressure would have to be 90% of the capillary pressure – which seems a lot. So, which is it? Or is it both?

In this study, experiments involving co- and counter-current spontaneous imbibition were conducted in precise model systems. Mineral oil was used to displace air. The pore space between parallel rods in a slot capped by a glass plate (so you can see what is happening) consisted of non-axisymmetric channels. These had angular corners, a bit like reals rocks. For any particular arrangement of rods, the tube geometry could be completely defined and fixed. So the capillary pressures could be calculated, and the hydraulic resistances could be measured or calculated. The experiments also tested Ruth's crossflow idea on co-current two phase displacement based on a bundle of capillary tubes. The results indicated what determined the back pressure in countercurrent imbibition so that Ruth's model could be applied to that situation as well.

Seeing if models behave like the real thing gave a better understanding of the imbibition process. This is of use to anyone trying to model imbibition using a pore network or continuum model, and also to anyone actually injecting water into a reservoir to get oil out. What we need to know is just what is the back pressure required to eject oil from rock? And how is it related to the capillary pressure of the rock? If the capillary back pressure is the major inhibitor then spontaneous imbibition could be increased by injection of short slugs of surfactant brine into a reservoir. These will flow through the fractures and, in transient conditions, will reduce the capillary back pressure at the fracture surface without reducing the capillary pressure in the rock. Oil should flow out of the rock into the fractures and ultimately out of the ground.

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Relating petrophysical models to geological interpretations—the Lucia method for carbonate formations

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ABSTRACT

Pore-scale models of various types are useful in hydrocarbon reservoir modeling for understanding the relationships between petrophysical properties, and for predicting difficult-to-measure flow properties from more easily measured properties in wells. However, constructing an effective three dimensional flow model for a subsurface reservoir requires much more than a prediction of flow properties along wellbores. It also requires an extrapolation of those properties into the much larger space between the wells where the only information available comes from seismic data and geological interpretation. This presentation does not address the topic of relating petrophysical properties to seismic data, but instead it is focused on the equally interesting and equally important topic of relating the quantitative world of petrophysical modeling to the descriptive world of geological interpretations.

One approach to linking petrophysical and geological models that has proven successful in carbonate reservoirs is the rock-fabric classification method of Lucia (1995). This method is based on a descriptive classification of the pore-space seen in thin sections involving observations of the relative amounts of grains, mud, and vugs, and if dolomite is present, the dolomite crystal size. The method includes empirical models relating the rock-fabric classification to interparticle porosity, vuggy porosity, permeability, acoustic velocity, and initial water saturation (Jennings and Lucia, 2003). At first glance it would seem that the use of a descriptive parameter with an arbitrary unitless scale would be a disadvantage in quantitative modeling of petrophysical properties, but it turns out that the rock-fabric classification is crucial for linking petrophysical and geological models because it is related to the only thing that does not vary rapidly along the depositional surfaces of many carbonate deposits—the depositional energy.

In this presentation the Lucia rock-fabric classification method will be introduced, and its porosity-permeability model will be compared to those of Winland-Pittman, Carman-Kozeny, and Bryant-Finney. The effectiveness of the Lucia model for predicting permeability laterally along depositional layers will be illustrated with data collected from an outcrop of the Permian Victorio Peak formation in West Texas.

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Pore-scale modeling of two-phase imbibition

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ABSTRACT

The interaction of different fluids in a porous medium is the result of the competition of different pore-scale displacement mechanisms. In the last 20 years, pore-network models have been used in order to simulate these pore-scale phenomena. During imbibition, three different mechanisms are described: piston–like, snap–off and cooperative pore–body filling. In this work a new model to describe the cooperative filling of a pore by the wetting phase during imbibition is presented. The new model is based on the local geometrical and petrophysical characteristics of each pore–body and its neighboring throats. Several sets of experimental data are used in order to validate the results of the new model. A very good match is found between the simulated and experimental results. Moreover, the results of the new model are compared with previous models results (stochastic models), showing that in general previous models tend to overestimate the trapping of the non-wetting phase during imbibition, while the new model describes more accurately the trends observed in the experiments.

Difference in wetting behavior of porous media with smooth and rough surfaces

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ABSTRACT

Work on the effects of surface roughness and pore structure on wetting by Wenzel (1936) and Cassie and Baxter (1944) is widely recognized as pioneering. Theoretical work on wetting of smooth parallel spaced rods was extended to three phase lines of contact perpendicular to heterogeneous striped wetting for planar surfaces (Cassie, 1948). Cassie's less-cited observations on the wetting of broccoli (1946) preceded what is now commonly called the lotus effect. Wenzel proposed a theoretical relationship between solid surface area and intrinsic versus effective contact angle. The relationship was first tested by Bartell and Shepard (1954) for machined pyramidal roughness. Measured effective contact angles could not be predicted from increase in surface area. Variation of advancing and receding contact angles from capillary rise in internally roughened tubes, for a wide range of intrinsic contact angles, showed wide variation in the Wenzel roughness factor which, according to the theory, should be constant. (Morrow, 1975). Controversy as to the validity of the Wenzel relationship is ongoing. One surprising development is that the work of Cassie and Baxter for a grid of smooth parallel rods has been identified by Marmur (2009) with trapping of non-wetting phase at rough surfaces, a condition previously depicted by (Huntsberger, 1963) in relation to wetting and adhesion. Raesi et al. showed that the MS-P method (Mason and Morrow, 1983) provides a powerful method of investigating surface roughness in all shapes of tubes of uniform cross-section, either closed or open.

Capillary drainage and imbibition pressures for porous media with controlled wetting correlated closely with change in receding and advancing angles measured at rough surfaces (Morrow, 1976); results were in distinct contrast to large decrease in imbibition pressure predicted for small increase in contact angle in pores formed by spheres because of converging/diverging pore shapes (Melrose, 1965).

For the complex mixed wetting conditions (Salathiel 1973) presented by clastic reservoir rocks containing connate water, the work of drainage combined with the efficiency of conversion of to surface free energy limits increase in surface area to 1/300th of the rock BET surface area (Brady et al., 2015). Water retained by surface roughness further limits the fraction of rock surface over which wettability alteration can occur by electrostatic interaction, likely by a further order of magnitude or more. The areas of close contact are mainly limited to surface asperities. In addition to capillary pressure, the corners and edges of surface asperities make a key geometric contribution to the disjoining pressure. For areas where the crude oil interface closely contours the rock surface, any changes in wettability by electrostatic interactions are almost instantaneous. Changes in wetting are not necessarily permanent. Spontaneous imbibition and waterflood data show that wettability alteration by crude oil exhibits reversible dependence on time and water saturation (Loahardjo et al., 2013). Reservoir wettability is not a fixed property.

Multi-phase lattice Boltzmann simulations of EOR mechanisms

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ABSTRACT

As part of a larger effort to develop and validate a two-phase Lattice Boltzmann simulator for typical EOR mechanisms such as changes in viscosity and interfacial tension, we present experiments and Lattice Boltzmann simulations of such EOR processes at the pore scale. Different EOR mechanisms have been imaged on the pore scale to capture the fluid distribution at residual saturations. This includes experiments of changes in fluid viscosity and interfacial tension. The same EOR mechanisms have been simulated by running Lattice Boltzmann simulations directly on images of the pore structure in question.

By image analysis of pore scale images we obtain the pore structure and distribution of the fluid distribution in the pore space. We further analyze such distributions by statistical measures such as cluster size distributions.

Both different boundary conditions and methods for changing fluid properties such as viscosity and interfacial tension have been investigated. Resulting residual saturations from such simulations have been compared to the experimental results to judge the applicability of the different boundary conditions, phase separation algorithms and methods for changing fluid properties. We use both direct visual observations and statistical measures, e.g. saturations and cluster size distribution, to compare the imaged experiments and the Lattice Boltzmann simulations at the residual saturations.

Level set approach for multiphase motion with isolated ganglia on the pore scale

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ABSTRACT

Understanding multiphase flow in porous media, including motion of isolated fluid ganglia, is important for increased oil recovery and CO2 storage applications in mature hydrocarbon reservoirs. Water-alternate-gas injections are processes that can mobilize and displace some of the residual oil in a reservoir after water flooding, but it can also lead to capillary trapping of gas. Core-scale measurements of trapped oil and gas saturations during water flooding show large variations that depend on pore geometry and initial saturations [1]. However, residual oil saturation is usually smaller in a three-phase flow than in a two-phase flow, but the total trapped gas and oil saturations can be larger, demonstrating gas-storage capacity. Micromodel experiments in two dimensions have shown that oil layers, located between gas and water, and double displacements, in which continuous gas and water displaces isolated oil, can lead to smaller residual oil saturations. However, it is important to perform three-phase experiments in 3D porous media and develop corresponding models to understand and predict three-phase trapping and mobilization mechanisms and the residual saturations.

We present a level set approach that combines multiphase methods for including contact angles [2], representing interfaces [3] and preserving phase volumes [4], and apply it to simulate three-phase capillary-controlled motion of disconnected gas and oil ganglia during alternate water and gas invasion processes in 3D pore geometries. We extend the approach to multiple displacement mechanisms in which two continuous fluids displaces several isolated fluid compartments. In water-wet rock, we observe frequently that water snap-off occurs along gas-oil interfaces due to water-cusp growth at gas/oil/water triple lines, which, depending on initial configuration and pore geometry, can initiate a double displacement and mobilize oil, or instead terminate a double displacement and capillary trap oil in water (see attached figures). We also observe that the disconnected oil can split into several ganglia, of which some trap permanently while others mobilize. The presence of a mobile, disconnected oil reduces the level of the gas/water capillary pressure curves. We calculate the isolated fluid-phase pressure and explain the motion by the pressure response during three-phase snap-off mechanisms and the pressure fluctuations during invasion into narrow and wide pore channels.

The snap-off mechanisms in our three-phase simulations share some similarities to the two-phase mechanisms observed in recent micro-CT imaging studies of “low, constant rate experiments” in real rock samples, which show cooperative behavior during drainage and imbibition [5, 6]. Motivated by this work, we propose, “volume targeting” in level set methods as a simple way to model constant-rate experiments. Instead of increasing capillary pressure stepwise and calculate saturation, we use the volume-preserving method [4] to specify target phase volumes, and then simulate quasi-statically a stepwise increasing saturation and calculate capillary pressures at each equilibrium. We observe Haines jumps with cooperative behavior, temporary snap-off events, and interface vibrations during the iterations needed to reach the specified saturation. Pressure fluctuations occur between equilibrium states and provides additional insights into the occurring mechanisms.

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On the history and applications of a perfect molar flow meter: Flux Response Technology

Presenter: Klaus Hellgardt
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ABSTRACT

Flux Response Technology was coined in the late 90'ies to describe a very sensitive pneumatic Wheatstone bridge to carry out molar balances on gas phase inventories. The origins of this technology can be traced back to the original work by Profs. Buffham and Mason, demonstrating the principle with nothing more than a manometer and a couple of tubes. Over the years the sensitivity of the technique has been improved to the point where volumes of mixing of gases can be detected and quantified. Many other applications have emerged since and have lead to multimillion pound support from Research Councils.
In this presentation I will highlight the numerous contributions Geoff Mason has made to the development of one of the most sensitive operando techniques currently available for gas sorption and diffusion measurements. I will explain how a humble pneumatic ensemble of tubes can be harnessed to measure complex dynamic behaviour of gas/solid, gas/liquid and gas/gas interactions. I will build the history of the development of the technique around the various applications that Geoff and others could envisage and conclude with an outlook on those applications that are still waiting to be discovered.

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GAS-PHASE DISPERSION ASSESSED FROM TRACER HOLDUP MEASUREMENTS ON A PACKED-BED - THEORY, APPARATUS AND EXPERIMENTAL TEST (OR HOW TO MEASURE DISPERSION WITH A PRESSURE GAUGE), ADDISON, PA, BUFFHAM, BA, MASON, G, YADAV, GD, CHEMICAL ENGINEERING SCIENCE, 49, 4, 561-572

Spontaneous imbibition of high and low salinity brine into a reservoir sandstone analyzed by micro-CT, microscopy and mineral mapping

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ABSTRACT

Coreflooding of clay-containing reservoir sandstones can yield substantial tertiary recovery by reducing the flood brine salinity, associated with a shift towards water-wetting. Spontaneous imbibition experiments, in which this salinity-induced shift is the main driver for additional recovery, can provide insight into the extent and source of the wettability change, especially when combined with pore-scale imaging of changes in residual oil configurations using micro-CT.

A homogeneous, friable, reservoir sandstone plug rich in kaolinite and illite/muscovite was solvent cleaned, from which two sister sub-plugs of 5 mm diameter and 18 mm height were cored. Each was similarly restored by saturation with its formation brine, primary drainage by centrifugation in crude oil to low irreducible water saturation, and ageing at 94ºC for 11 days. To explore the influence of crude oil composition, each plug used a different oil, of similarly low density, viscosity and asphaltene content, but primarily distinguished by their acid numbers of 3 and <0.1 mg KOH/g oil. Spontaneous imbibition of seawater was performed at 94ºC for 7 days, followed by cooling to room temperature and diffusional ion exchange for seawater doped with 0.4 M sodium iodide for 3 days to boost X-ray attenuation contrast between oil and brine. Each sub-plug was helically micro-CT scanned over its entire height at 2.3 µm/voxel. After re-exchange of the contrast brine for seawater, the above-mentioned procedure of spontaneous imbibition, ion exchange and scanning was repeated using a low salinity brine comprising 500 ppm sodium chloride. These two tomograms for each plug, together with reference tomograms of both their re-cleaned and contrast-brine saturated states, were spatially registered to exactly overlay each other. This facilitated segmentation of solid grains from clay aggregates, and of oil from brine occupancy within resolvable and sub-resolution pores.

Analysis of these segmented tomograms showed that both sub-plugs possessed very high residual oil saturation (around 93%) after exposure to the high salinity brine, implying a substantially oil-wet state. Subsequent exposure to low salinity brine resulted in a large tertiary recovery by spontaneous imbibition, which reduced oil saturation by 14 and 11 p.u. for the high and low acid number oil, respectively. The tomograms were further analyzed to quantify the salinity-induced pore-scale changes in oil saturation in resolvable and sub-resolution pores, oil inter-pore connectivity, oil-grain and oil-clay interfacial areas and oil-brine interfacial area and mean curvature. Additional insight into the origins of the apparent shift to more water-wetting were obtained by preparing polished embedded sections of the sub-plugs for higher resolution BSEM imaging and SEM-EDS mineral mapping. These 2D images were registered into the corresponding cross-section of the 3D tomograms of each sub-plug. In this way the salinity-induced release of oil could be overlain and directly compared to the mineral originally contacting it at each location.

Prof. Mason's impact on recent advances in pore scale modeling

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ABSTRACT

Accurate representation of geometry has the first order influence on multiphase fluid flow in porous media (and more) on all relevant scales. On the nanometer to millimeter scale, complex void space features are notorious for dictating macroscopic fluid flow due to dominant capillary forces. Dr. Mason’s work pioneered now traditional approaches in pore scale modeling of fluid displacement as well as sorption. I will briefly review the pore scale modeling approaches of fluid displacement in my research work that relate to Dr. Mason’s work. These range from the level set method based models of interface displacement in model soils or propped fractures, to quasi-static pore network models of displacement as well as sorption, and most recently to using Dr. Mason’s work as the basis for multiscale pore network modeling of tight/unconventional media. The common thread in these seemingly different approaches is that the originating geometry is modified from the same sphere packing used by Prof. Mason.

The Real Reason Why Sodium Explodes in Water

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ABSTRACT

Geoff Mason was my Father, and we often talked together about our scientific research. One of the more bizarre things that I was interested in, was the sub-millisecond explosion of sodium in water, primarily because it just should not happen. You have alkali metal, and water, and they can only react on the interface, and when they do they generate alkali hydroxide and hydrogen, both of which should keep the reagents separate and prevent further reaction, so how can it explode in less than a millisecond? One rather interesting suggestion supported by several lines of evidence was that the force that drives alkali metals to explode in water is columbic in nature.[1] During the last months I spent with my Dad, we had some very interesting discussions about the problem, and even did some remarkably 'Geoff' type experiments to test his ideas. This ones for you Dad!

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Temperature rise at an imbibition front

Presenter: Majid Hassanizadeh
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ABSTRACT

Spontaneous imbibition of a wetting phase into a porous medium is believed to be driven by energetic forces. The nonwetting phase-solid interface is known to have a higher interfacial energy than the wetting phase-solid interface. Thus, the imbibition process is expected to lead to the release of energy and thus a rise of temperature at the front. In order to investigate the occurrence of this effect, experiments were performed involving the penetration of water into three different paper types (Plain, glossy and plastic based). A thermometer with accuracy of 0.1 ºC was firmly attached to a position away from the inlet area. First water and paper were brought to the room temperature. Then, water was injected to one end of a strip of paper. The temperature was found to rise gradually as the water front approached. The temperature rise was 0.6, 0.5 and 0.2 ºC for plain, glossy and plastic based papers.

What can we learn from spontaneous imbibition curves?

Presenter: Martin Fernø
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ABSTRACT

Key scientific questions covered in the talk

Is the rate of oil recovery from spontaneous imbibition always linear with the square root of time?
In our experimental studies we find that this is not the case. Although a common assumption is that the rate is linear with square root of time, we have shown experimentally that the rate of water imbibition, and subsequent oil recovery, depends strongly on the applied boundary condition. We also know from experiments that counter-current imbibition is not always square root of time, and these cases will be reviewed.

What forces are dominant during spontaneous imbibition?
The capillary pressure is the dominant driving force for the spontaneous imbibition process. A key question is to identify the resistance forces, and to evaluate if, and how, these change over time. A review of recent experiments that probe this will be presented.

Can we learn more from a simple spontaneous imbibition experiment?
Recent advances with applied boundary conditions will be discussed in detail and new key insights to measuring parameters that act during spontaneous imbibition, namely the capillary pressure and relative permeability, will be reviewed.

What does visualization bring to the table?
Access to changes in local fluid saturations during a dynamic displacement test significantly increase the information gained from such displacement processes. A newly adopted positron emission tomography imaging approach will be reviewed and examples from spontaneous imbibition will be presented.

How to best design your spontaneous imbibition test?
Based on experimental experience of the past decade, this talk will provide insight into some key aspects related to preparation and executing a successful spontaneous imbibition test.

Curvature Measurement, Nonwetting Phase Trapping and Film Flow in Porous Media

Presenter: Dorthe Wildenschild
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ABSTRACT

We use x-ray microtomography images to predict capillary pressure of fluid-fluid interfaces via interfacial curvature measurement and use of the Young-LaPlace equation. Several improvements have been made to previous algorithms by removing interface segments that are affected by proximity to the solid surface, and by using distance-weighted curvature estimates. The new algorithms show significant improvement over previous quantification and allows for a close match to externally-measured capillary pressure values obtained using pressure transducers.

Importantly, the data also allows us to track the pressure state of trapped nonwetting phase and 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.

Quantitative pore capillary pressure functions for network modeling

Presenter: Karsten Thompson
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AUTHORS

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ABSTRACT

Imbibition and drainage exhibit a variety of interesting behaviors that are influenced by the movement and configurations of fluid-fluid interfaces in individual pores. The fundamentals of these pore-scale processes are well understood due to years of research on this topic. However, quantitative modeling of fluid-fluid interfaces at the pore scale remains challenging. The situation as it applies to pore-network modeling is of particular interest: whereas modern pore-network modeling is often based on microtomography images (very detailed descriptions of pore geometry and topology), network modeling is attractive because of its relative simplicity and computational efficiency. In this work we explore a new technique that balances the ability to obtain detailed interfacial phenomena with the desire to maintain a high level of efficiency with pore network modeling. This solution is obtained through the use of pore capillary pressure functions, which describe local capillary pressure as a function of local saturation. They are unique to each pore and differ significantly in functionality from continuum scale capillary pressure functions. The local functions are quantified using digital images of the pore structure by probing the pore-space with a set of computationally generated test spheres. The information is then translated into a spatial field of the total interfacial curvature. Finally the distribution of curvatures found in any given pore (discretized on the digital image) is mapped back to a pore capillary pressure function that can be used in multiphase pore network models. This approach incorporates a rich set of information about local interfacial behavior without the computational demands associated with direction numerical simulations that perform interfacial tracking.

Studies of Snap-off in Triangular Microfluidic Devices

Presenter: JIA YAO
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ABSTRACT

Oil reservoir rock is typically a porous medium consisting of interconnected microscale pores and throats. The pore-throat geometry of any individual reservoir can vary widely, based upon differing sizes and arrangements of sediment grains. To create simplified proud geometries as experimental models, capillaries and tubes with circular or rectangular cross-sections are often utilized. Microfabricated fluidic platforms also provide excellent representations of microscale porous media and have been widely utilized for the direct visualization of multiphase flows. These so-called micromodels have been fabricated with reservoir rock-patterned channel networks and used to investigate two-phase water-oil flow processes. However, microfluidic fabrication technology limits the options of available cross-sectional geometries that can be produced to rectangular or rounded-rectangular troughs. To overcome this limitation, we have introduced ultrafast pulsed laser direct writing to quickly produce channels with arbitrary cross section. Simultaneous spatial and temporal focusing (SSTF) femtosecond pulsed laser systems were used to directly write channels in glass with triangular cross-sections. This approach surpasses planar lithography in speed and flexibility, while providing the ability to vary depth within individual channels. We have employed triangular channels of arbitrary cross section to examine the influence of geometry on oil-brine snap-off, which is a determining phenomenon in enhanced oil recovery (EOR) processes. Comparisons between rectangular and triangular cross-section channels illustrate the significant influence of geometry on snap-off. Experimental results for varied geometries are analyzed in the context of the Mayer and Stowe and Princen (MS-P) theory, which allows for the calculation of capillary pressure and meniscus curvature in microscale capillaries of uniform cross section. This work validates MS-P theory for triangular channels and establishes a new class of micromodels for hypothesis-driven EOR studies.

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Surface complexation and two phase lattice Boltzmann modelling

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ABSTRACT

In order to investigate the impact of carbonate surface charge on carbonate dissolution kinetics, van Cappelen et al. (1993) [1] used a surface complexation model. Hiorth et al. [2] extended this work to account for sulphate complexation, and the HKF equation of state (see e.g. Oelkers et al 1993) was used to predict the temperature dependency of the surface complexes. The variation of the surface potential as a function of temperature was investigated in order to clarify how oil recovery correlated with surface charge and calcite dissolution. A similar approach was later used by Brady et al. [2] for adhesion of polar oil components to minerals, and to relate these surface complexations to oil recovery. Mahani et al. [3] also used surface complexation modelling to interpret zeta potential measurement on calcite, limestone, chalk outcrop and dolomite outcrop.
All of these models only consider the interaction between a mineral surface and organic molecules and/or ions dissolved in the water. However, in order to relate local changes at the pore surface such as surface charge, dissolution/precipitation and surface complexation to oil production, it is necessary to include these reactions in pore scale simulations. In this paper, we extend the standard Shan-Chen lattice Boltzman model [6] for multiphase flow to account for surface complexation reactions. We calculate the change in Gibbs free energy using the Chan-Mitchell charging process [7], and relate this to changes in the oil/water contact angle. We study the change in contact angle as a function of the brine chemistry and discuss this in the context of laboratory experiments.

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Pore network modeling of capillary hysteresis in neutrally wettable fibrous media

Presenter: Jeff Gostick
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ABSTRACT

Pore network modelling was used to simulate primary and secondary drainage and imbibition in neutrally wettable fibrous media used for fuel cell electrodes. Excellent agreement was found between experimental air-water capillary pressure data and the numerical simulations when using the Purcell toroid model explored by Mason and Morrow in 1994. Without this model the experimental data are impossible to rationalize both in terms of the observed capillary pressures, as well as the apparent change in wettability between water injection and withdrawal. The calibrated network model was then used to simulate gas phase diffusivity through partially water-saturated materials which is of relevance to fuel cell operation.

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Application of a multi-scale form of Terzaghi's effective stress principle for unsaturated expansive clays to simulate hydro-mechanical behavior during hydration

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ABSTRACT

Our multi-scale approach of Terzaghi's effective stress principle for unsaturated swelling clays that was rigorously derived by homogenization starting from micro- and nano-mechanical analyses [1] is applied to numerically simulate oedometric swelling pressure tests on compacted bentonite samples during hydration [2,3]. The macroscopic total stress of our model captures the coupling between disjoining forces at the nano-scale of the clay platelets and capillary effects at the micro-scale of the clay aggregates over the entire water content range. The numerical results allow thus conclusions about water transfer between inter- and intra-aggregate pores during hydration and thus about the evolution of the external swelling pressure resulting from the competition between capillary and disjoining forces.
In addition, this application highlights the abilities and the limits of the electrical double layer theory to compute the disjoining pressure in the nano-pores. For large distances between the platelets, in the so-called osmotic swelling, the disjoining pressure is of electro-chemical nature and results from the solution of the Poisson-Boltzmann problem. At small distances, on the contrary, in the crystalline swelling, it seems necessary to add a solvation component due the molecular nature of the water. As a first improvement of the nano-scale description the solvent thus is treated as a simple hard sphere fluid confined between two planar hard walls using Density Functional Theory.

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Micro-mechanics of unsaturated granular media with interfaces

Presenter: Jerome Duriez
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ABSTRACT

The present work is concerned with an analytical derivation of the stress tensor expression for unsaturated granular materials based on homogenization. In contrast to other works that advocate thermodynamics for the description of the various phases and their interactions, we herein use an alternative approach which provides the explicit treatment of micromechanics and statistical aspects. More precisely, we consider a three-phase mixture that includes distinct solid particles penetrated by a wetting fluid (w) and a non-wetting one (n). The novelty here is that the expression of the total stress for the mixture accounts for the 3 different bulk phases, as well as the associated interfaces endowed with specific energies and a surface tension force field. As such, specific interface stress tensors together with appropriate boundary conditions for the solid stresses enter the derivations. Interestingly, it is found that the contributions of the two solid-fluid interfaces, i.e. s-w and s-n, are zero.
The above-mentioned homogenization approach is applied to the case of an idealized granular assembly where polydispersed spherical particles are connected by liquid bridges in the so-called pendular state. Such an unsaturated granular medium can also be analyzed using the Discrete Element Method (DEM) where, instead of explicitly computing pore fluid physics, a uniform suction is assumed throughout the assembly and as such the capillary force and associated geometry of the liquid bridge can be calculated from Laplace-Young's equation. Here, the action of every liquid bridge on the solid phase is conveniently replaced with a resultant capillary force that is added to existing inter-particle forces that are mechanical in nature. Thus, for a given suction and wetting (contact) angle, a DEM computation of an unsaturated granular assembly allows us to have access to a large variety of microstructural information such as liquid bridge distribution, particle packing, including interface characteristics such as surface areas and wetted perimeters. Using the analytically derived averaged stress expression, the validity of the DEM approach in treating liquid bridges and interfaces through a resultant force on solid particles is explored.
Another important outcome of this study is the non-spherical nature of the capillary or suction stress, in the terminology of Lu & Likos (2006), that describes stress contributions from the different fluid phases and the interfaces. In fact, it is recognized that the capillary stress has a deviatoric component following the fabric of the granular material and contributions from interfaces. This distinction from classical theories (e.g., Bishop, 1959) where suction is considered to be isotropic is essential to the understanding of unsaturated pendular state granular material behaviour. Interestingly, it is found that the interface contribution to the capillary stresses is significant in the pendular regime, excluding very low saturation, see the attached Figure.

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Consistency Requirements in the Modelling of Coupled Hydro-Mechanical Behavior of Unsaturated Soils

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ABSTRACT

Nearly all elasto-plastic models for unsaturated soils were developed for deformable unsaturated soils. In these soils the mechanical and the hydraulic behavior of the soils are coupled together. For example, applying an external load to an unsaturated soil can result in a decrease in the volume change of the soil skeleton. Volume change of the soil skeleton will cause changes in the matric suction. Changes in the matric suction again will cause volume change in the soil skeleton. The final results depend on the coupling effects among the soil skeleton, the water phase and the air phase. During this process, there may be irrecoverable changes for the soil. The first elasto-plastic model for unsaturated soils was proposed by Alonso et al.(1990). The model was later referred to as the Barcelona Basic Model (BBM). In the BBM, the elasto-plastic model was developed for the soil skeleton only. The behavior of the water phase was represented by a unique degree of saturation versus suction curve and essentially elastic. Wheeler and Karube (1996) pointed out that in the BBM the models for the soil skeleton and the water phase were inconsistent and cannot be used for fully coupled hydro-mechanical analyses. Since then many researchers developed elasto-plastic model for unsaturated soils in which special attention was paid to the modeling for the water phase. Review of elasto-plastic models for unsaturated soils can be found in Gens (1996), Delage and Graham (1996), Wheeler and Karube (1996), Vanuat (2005), and Gens et al.(2006).
Although attention was increasingly paid to the coupling effect between the mechanical and hydraulic behavior of unsaturated soils, little work was done to consider compatibility among the elasto-plastic models for the soil skeleton, the water phase, and the air phase. This paper discusses the consistency requirements in the modelling of coupled hydro-mechanical elasto-plastic behavior of unsaturated soils. The BBM was used as a representative to demonstrate how to use the MSSA to modify an existing model to simulate the coupled hydro-mechanical behavior for unsaturated in a consistent way.

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Multiscale characterization of laminated sandstone intervals

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ABSTRACT

Laminated sandstone intervals frequently host significant hydrocarbon reserves, yet their reservoir properties including porosity, permeability, capillary pressure and saturations) are highly variable and difficult to predict. It is also not clear how they should best be represented in either static or dynamic models. In this paper we describe the application of a multiscale 3D imaging study to better describe the reservoir properties of a laminated sandstone sample from a CO2 demonstration project. The project included acquisition of >60 m of whole core from a single well, the choice of >20 plug samples from whole core scanned regions and acquisition and image registration of pore scale samples from different rock types within the plug volumes. Continuous flow measurements were also undertaken at the whole core scale via point-focus physical properties scanning of whole core. This large data set offered a unique opportunity to test the value of digital core techniques for carbon sequestration assessment and to model the enormous range of scales encountered in a complex laminated sandstone—spanning from the pore space (microns) to whole core (meter lengths). Key steps in the successful application of the program included improved whole core scanning which enables one to provide a quantitative bridge from plug scale measurement to meter scales, developing methods to consistently and robustly identify important sedimentary features at larger (coarser resolution) scales and the development of improved classification schemes along continuous lengths of core. The outcome of this program shows that digital rock technology results can be consistent with laboratory and model whole core data on complex laminated sands. It also enables one to investigate the range of possible outcomes of CO2 plume movement in the storage reservoir, as a function of injection rate and depth, by incorporating known contributors to uncertainty (small-scale heterogeneity) that, to date, have not been incorporated into larger scale storage site-scale static models. Future work on the project will also be discussed-- particularly incorporating outcrop descriptions, sedimentary features and log data (e.g., investigate the role of different lamina -- parallel and cross beds) to the upscaling study.

The Impact of Pore structure and Surface Roughness on Capillary Trapping for 2D- and 3D-porous media: Comparison with Percolation theory

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ABSTRACT

We study the impact of pore structure and surface roughness on capillary trapping of non-wetting gas phase during imbibition with water for capillary numbers between 10^-7 and 5 x 10^-5, within glass-beads (GBS), natural-sands (NS), glass-beads monolayers, and 2D-micromodels (see Fig. 1). The materials exhibit different roughness of the pore-solid interface. We found that glass beads and natural sands, which exhibit nearly the same grain size distribution, pore size distribution and connectivity, showed a significant difference of the trapped gas phase of about 15%. This difference can be explained by the micro-structure of the pore-solid interface, i.e. the surface roughness. Our main conclusions are:

(1) Geometrical Similar Porous Media having the same Wettability can show a significant difference in Capillary Trapping Efficiency
The experimental results (micro-CT) reported in this study support our working hypothesis, namely that the trapping process in 1mm-GBS- and 1mm-NS-packs, which possess nearly the same grain size distribution, pore size distribution and connectivity, is completely different: by-pass trapping governs the capillary trapping process in glass beads, while snap-off trapping governs the capillary trapping process in natural sands. Moreover, the results of the visualization experiments of 1mm-GBS-monolayers and 2D-micromodels explain the large difference in trapping efficiency of approximately 15%, when comparing 1mm-NS with 1mm-GBS.

(2) The Transition Zone Model can be applied to Ordinary Bond Percolation with Snap-Off Trapping within 2D-Micromodels with Rough Surfaces
Therefore, it can be expected that the experimental cluster size distribution at small capillary numbers(about 10^-6) shows universal power-law behavior. The visualization experiments of 1mm-GBSmonolayers verified the usual transition zone model, i.e. by-pass trapping was observed within the width of the rough interface. The observed universal scaling behavior is a strong argument that at the bottom of this transition zone the trapped gas phase is at its percolation threshold. For the first time it is demonstrated experimentally that the transition zone-model (invasion percolation within a gravitational gradient, mean field approach [Wilkinson, 1984]) can be applied to 2D-micromodels, if bicontinuity is generalized such that it holds for the thin-film water phase and the bulk gas phase.
Based on our experimental results we conclude that invasion percolation describes the capillary trapping in 1mm-GBS-packs and ordinary bond percolation the capillary trapping in 1mm-NS-packs. The universal scaling behavior of the cluster-size distribution observed in both 3D-porous media supports this picture.

Figure 1 Trapping efficiency for 2D- and 3D-porous media. The black symbols represent own experimental results [Geistlinger et al., 2015a,b; Geistlinger and Mohammadian, 2015c] and the colored symbols selected results from literature.

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3D connectivity metrics to describe multiphase fluid flow characteristics and porous medium structure

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ABSTRACT

The distribution of nonwetting phase fluid as it flows through a multiphase fluid-porous medium system has dramatic impacts on nonwetting phase transport properties and trapping behavior, with great relevance to subsurface engineering applications (e.g. oil recovery, geologic CO2 sequestration, environmental remediation, etc.). In the attempt to describe fluid distributions, considerable effort has been made to characterize flow regimes of nonwetting phase as a function of various fluid, flow, and medium properties from a two-dimensional (2D) perspective [e.g. 1–3]. However, flow pattern discrimination in three dimensional (3D) systems has proved more difficult, partially due to the difficulties inherent in non-destructively imaging dynamic fluid flows in 3D samples at relevant spatial and temporal resolutions; and partially due to the inherent difficulties associated with characterization of 3D fluid flows (i.e., in contrast to 2D systems, 3D fluid flows are often visually too complicated to easily discern patterns).
We present qualitative and quantitative descriptions of 3D fluid flows measured from a suite of core flooding experiments in a variety of porous media (glass bead columns as well as Bentheimer, Berea, and Leopard sandstone cores) and under different flow conditions. Fluid and solid distributions are characterized via x-ray microtomography, which provides for precise and accurate characterization of pore-scale fluid-fluid-solid interfaces and distributions; and we have utilized experimental protocols which allow for high-resolution, low noise tomographic scan collection at discrete time intervals during flow processes (drainage and imbibition). From these 3D data volumes, we calculate quantitative connectivity metrics of the nonwetting phase as it evolves during drainage and imbibition flows, using metrics derived from statistical percolation and mathematical topology. In addition, we use novel quantitative metrics to investigate the inherent geometry and connectivity of the porous media and relate this to the nonwetting phase transport. The results provide insight into the flow regimes and trapping behavior of fluids in these systems, and highlight new quantification tools which can be used to characterize 3D solid structures and fluid flows.

Graphic 1: Vertical slice through a 3D x-ray tomographic grayscale volume depicting air (dark gray) intrusion into Bentheimer sandstone (moderate gray) which was originally completely saturated with brine (light gray).

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Scaling Effect of Shear Modulus of Unsaturated Soils from Small-Strain to Finite-Strain

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ABSTRACT

Soil has been known by its nonlinear stress-strain relationship. The shear modulus of soil degrades as the strain level increases. A hyperbolic model can describe this shear modulus reduction behavior. For unsaturated soils, two mechanisms have been conceptualized to define the scaling effect as the modulus reduces from small-strain level to finite-strain level. A redefined modified-hyperbolic model was proposed to capture the differences between small-strain and finite-strain shear modulus as the soil moisture changes. The small-strain shear modulus represented by the shear wave propagation is a process of local small disturbance transporting through the soil skeleton within the elastic range, whereas the finite-strain shear modulus represented by static loading is a accumulation process of local large disturbance and diffusion with time. Two parameters were introduced to quantify the scaling effect: reference strain indicating a threshold of the strain level where the shear modulus reduced to half of its small-strain modulus; a power of the dimensionless strain ratio reflecting the different developing patterns of small-strain and finite-strain shear modulus with water content dependency. These two parameters are depended on soil type and have close correlation with soil water retention of the soils. The correlation between reference strain and pore size distribution parameter of soil water retention suggests that the capillary water dominates the finite-strain shear modulus development. On the other hand, correlation between the power exponent and the adsorption water capacity reveals that the fine soil content or the adsorption water plays an important role for the small-strain shear modulus. Finally, using the proposed shear modulus reduction model and its correlation with soil water retention, given one of the small-strain or finite-strain shear modulus can predict very well the other counterpart with varied degrees of saturation.

A mechanistic interpretation for the variability of rainfall-induced landslides based on unsaturated porous media principles

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ABSTRACT

This contribution discusses the role of coupled hydromechanical processes on the stability of unsaturated shallow slopes subjected to transient water infiltration. In particular, the role of capillarity-induced cohesion, water retention characteristics, and suction-hardening properties have been explored by introducing a simple rigid-plastic constitutive model for the solid skeleton. The objective is to develop analytical expressions for Factors of Safety (FS) for two types of slope failures commonly known in literature: slow-moving frictional slips, and fast-propagating flowslides. These failure indices have been derived by identifying the conditions for loss of uniqueness and/or existence of the deformation/wetting response predicted by the proposed rigid-plastic model [Buscarnera, 2014] and combined with the initial stress state within an infinite slope. The obtained expressions suggest that such hydromechanical processes play a considerable role on the critical stress ratios associated with failure, affecting the values of safety factor for all the failure mechanisms under consideration, providing thus a mechanistic interpretation of the variability of failures scenarios often observed at the regional scale. To test their predictive capabilities, these FS have been assessed against literature data for flume tests on highly liquefiable soils, effectively capturing the observed different failure modes associated with distinct initial conditions. Finally, they have been combined with hydrologic models and incorporated into a Geographical Information System (GIS) platform to capture the spatial and temporal patterns of slope failures at a regional scale, thus illustrating the possibility to enhance current landslide-susceptibility modelling strategies by encompassing principles of unsaturated porous media.

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Effective Stress Evaluation of Undrained Compression of Unsaturated Soils

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ABSTRACT

This paper focuses on an effective stress evaluation of the compression response of unsaturated soils during undrained compression. During undrained compression of unsaturated soils, the void ratio, degree of saturation, pore air pressure, pore water pressure, and compressibility are expected to change in different ways. A modified form of Hilf's equation is combined with the isotropic stress-strain curve in terms of effective stress to predict the changes in. These results are compared with the results from undrained compression tests on unsaturated, compacted clay. The modified form of Hilf's equation and the effective stress analysis are found to provide a superior explanation of the compression response of unsaturated soils as compared to a conventional total stress evaluation using Hilf's equation.

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The migration of fine particles as a new approach to explain the mechanism of soil collapse.

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ABSTRACT

: Collapsible soils are unsaturated soils which present important potential deformations after damping with or without loading. Thus the subsidence due to the collapse of the soils can pose serious problems, as well to existing works as new constructions. For this purpose, the present paper consists of the study of the behavior of collapsible samples subjected to various hydraulic loads of saturation and various vertical loads, with an aim of studying and clarifying the effect of these two parameters on the collapse potential of the soils. The results obtained show clearly that the subsidence of collapsible soils reach the maximum for a load of 400 kPa and the displacement “erosion” of the fine particles of a horizon to another through the soil matrix is one of the mechanisms of collapse.

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Continuum-scale simulation of two-phase flow micro-model experiments

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ABSTRACT

Two-phase flow micro-model experiment[1] is simulated as 1-dimensional problem at Darcy-scale. Extended Darcy's law with wetting/non-wetting phase interfacial area is adopted[2][3][4][5]. Saturation distribution, interfacial area velocity from simulation is compared with experimental drainage and imbibition data.

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An Optical Method to Measure the Total and Localized Volume Changes of Unsaturated Soil Specimens during Triaxial Testing Under Different Confining Pressures

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ABSTRACT

Triaxial tests have been widely used to evaluate the soil behavior. In the past few decades, several methods have been developed to measure the volume changes of unsaturated soil specimens during triaxial tests. Literature review indicates that until now measuring the volume changes of unsaturated soil specimens during triaxial testing remains a major challenge for researchers.

A noncontact method is developed to measure the total and local volume changes of unsaturated soil specimens using a conventional triaxial test apparatus for saturated soils. The method is simple and cost-effective, requiring only a commercially available digital camera to take images of an unsaturated soil specimen during triaxial testing from which accurate 3D model of the soil specimen is reconstructed. In this proposed method, the photogrammetric technique is utilized to determine the orientations of the camera where the images are taken to an accuracy to 3 microns, multiple optical ray tracings are employed to correct the refraction at the air-acrylic cell and acrylic cell-water interfaces, and a least–square optimization technique is applied to estimate the coordinates of any point on the specimen surface. Validation tests indicated that the accuracy for the point measurements is 76 microns in the water and less than 0.25% for total volume measurements. Methods are also developed to calculate the total volume and localized strains based upon the 3D discrete measurement points on the specimen surface.

The procedure of the proposed method as follows: (1) first some measurement targets are posted on the load frame, acrylic cell, and surface of the soil specimen (Figure 1a); (2) a commercially available digital camera (Figure 1b) is used to take many photos around the whole system (Figure 1c). The camera positions could be arbitrary. (3) A computer program developed based upon the proposed method is used to reconstruct the 3D images of the cell and the soil specimens (Figure 1d) from which the total volume and localized strains (Figure 1e), especially the shear band can be computed.

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Three-dimensional experimental and numerical study of heat and mass transfer through unsaturated porous media

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ABSTRACT

It is well known that the heat and mass transfer are coupled in unsaturated soils. A large body of experimental observations are available either confirming the movement of moisture under non-isothermal conditions or quantifying the importance of thermal gradients on moisture transfer. As the study of coupled heat and mass transfer is gaining attention in a number of practical engineering applications (e.g., soil borehole thermal energy storage systems, buried high-voltage electrical cables, waste disposal, etc.), the need for high quality experimental data is also growing. Precise experimental data can be used to validate numerical models and test the theoretical formulations of physical processes. This work is aimed at better understanding of effects of dimensionality, domain heterogeneity and boundary conditions on heat and mass transfer through unsaturated soil. This study provides robust 3D laboratory data at the intermediate scale that can be used to evaluate different assumptions/parameterization during numerical model validation. In this study, a 3D fully coupled numerical model that solves for heat, liquid water and water vapor flux and allows for non-equilibrium liquid/gas phase change was tested. Four intermediate scale (210×120×60 cm) laboratory experiments were performed under varying thermal (70 and 80 °C) and saturation conditions in an effort to simulate soil borehole thermal energy storage environments. Soil moisture and temperature were continuously monitored throughout the tank. Numerical results showed that under the test conditions used in these experiments, convective heat fluxes are higher compared to the conductive fluxes indicating that moisture flow (either in liquid or vapor form) has more contribution to the overall heat flux than conductive fluxes for the conditions tested. This finding is important in soil thermal energy storage systems as the common modeling practice is to assume that heat is only transmitted through conduction.

Modeling freezing-thawing cycle of frozen soil at the finite deformation range

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ABSTRACT

We investigate the freezing-thawing effect of frozen soil using a stabilized thermo-hydro-mechanical (THM) finite element model. By applying mixture theory, frozen soil is idealized as a composite consistent of four phases, i.e., solid grain, air, unfrozen water and ice crystal. A generalized hardening rule is adopted to replicate how critical state evolves under a combination of non-mechanical loading, such as degree of saturation, temperature and phase transition. The enhanced particle interlocking and ice strengthening, and the cryo-suction effect in frozen soil are replicated. Meanwhile, mass-exchanges among constituents due to phase transition are considered. A stabilized equal-order finite element model that employs mass, momentum and energy balance laws as governing equation are used. Inf-sup tests are conducted to ensure the spatial stability of the numerical models. The frost heave problem and triaxial compression tests at different temperatures are used to benchmark and validate the numerical schemes.

Novel Processing and Characterization of Cellulose Nano-Composite made from Improvised Liquid Composite Molding Process

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ABSTRACT

Abstract
The plant-derived cellulose nano-fibers (CNF) are increasingly used as a reinforcement for polymer composites due to their high modulus and potential for sustainable production. In this study, CNF/epoxy nano-composites were made from CNF aerogels being used as a preform through an improvised Liquid Composite Molding (LCM) process and characterized to determine the influence of the micro porous structure of CNF aerogel on mechanical and tribological properties of bio-based epoxy composite. Formation of the CNF preform during its processing strongly affects the global mechanical properties of the composite, therefore mechanical testing was performed to characterize the influence of isotropic and anisotropic pore structure on the final properties. The causes of mechanical failure were investigated through analysis of fracture surfaces using SEM.

Keywords: Cellulose Nano-fibers, CNF, LCM, natural composites, isotropic and anisotropic pore structure.

1. Introduction
Polymer composites are increasingly used in several sectors of engineering such as automotive, aerospace and construction in recent years. Growing environmental awareness has enhanced interest in the use of environmentally low-impact materials in engineering [1]. Cellulose nanofibers (CNFs), a new type of nanofibers made purely of cellulose molecules, have very good mechanical property compared to other natural fibers, and are comparable even to carbon or glass fibers [2-4].
Aerogels are an extreme light-weight and porous materials that are made by removing liquid solvent from a gel, as a result of which a solid skeleton is created with large spaces between the solid phases [5]. Formation of aerogels is usually accomplished through common processes including freeze- and vacuum-drying processes. Cellulose is an attractive material to make aerogels from due to its high availability and biodegradability (Figure 1).
In the present study, we use the porous CNF aerogel as a reinforcement with an epoxy matrix. The idea was that cellulose nano fibers present in the CNF skeleton bond with the matrix in order to create three-dimensionally disbursed system of nanoparticles thus creating an effective nanocomposite. The composite was made using a unique vacuum-suction driven liquid composite molding (LCM) process. The mechanical behavior of the resulting CNF composite (or nanocomposite) was evaluated experimentally.

Figure 1. Cross section of a CNF preform showing (a) randomly oriented and (b) highly aligned pores

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The Non-Newtonian Behavior of Automatic Transmission Fluid through Porous Media at Subzero Conditions

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ABSTRACT

In the filtration industry, the Darcy's law is being utilized to theoretically calculate the pressure drop of fluid flow through porous media. This equation is widely used as an engineering tool for designers to dimension filters for transmission systems. One of the most important design criteria very often involves to meet pressure drop requirement at subzero conditions. Discrepancies as high as 40% between test data and Darcy based computational results were observed, especially at cold temperatures.
The objective of this work was to determine the root cause of this disagreement. Media compressibility effect as well as icing effect were considered in this investigation. This work presents test data on pressure drop measurements between -15C and -35C using a Mercon series automatic transmission fluid. Two type of porous materials with same effective areas were utilized, a felt media and a metal mesh. Both of these were subjected to same volumetric flow condition. Finally, two more cases are presented for discussion, a metal cylindrical tube and a single layer media filter.
These experimental data showed a consistent fluid behavior in all of the tested media, including tube and filter. All of them showed a higher than calculated pressure drop values at cold temperatures. Normalized pressure values confirmed the calculated apparent viscosity, for a given subzero temperature and flow rate, is higher than expected in all cases giving similar relative values. Same fluid behavior was observed when viscosity measurements were conducted at different shear rates using a modified Brookfield method. The apparent viscosity dependence of not only the temperature but also the flow shear rate indicates the non-Newtonian behavior of the automatic transmission fluid at subzero conditions.

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Simulation of vacuum-assisted resin transfer moulding (VARTM)

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ABSTRACT

Resin transfer moulding (RTM) is a common manufacturing procedure for complex-shaped structures made of fibre-reinforced materials, such as carbon-fibre-reinforced plastics (CFRP) or glass-fibre-reinforced plastics (GFRP). The RTM-process set-up is composed of a rigid two-piece casting mould. The dry (gas saturated) fibre fabric is placed in the mould and is thereafter compressed by its matching counterpart. Following this, the resin is injected at the inlet via an excess of pressure subjected to the resin. The resulting pressure gradient between the inlet and the open (ambient-pressure exposed) outlet, initiates a resin flow which gradually impregnates the fabric. Finally, the fully resin-saturated part is cured.
One of the major drawbacks of the RTM method is its need of a two-piece casting mould, which is expensive, especially when large structures are manufactured. To cope with this, the method of vacuum-assisted resin transfer moulding (VARTM), often also denoted as vacuum-assisted resin infusion (VARI), has been developed. Therein, in contrast to the RTM process, the procedure set-up is composed of single-piece casting mould and a flexible plastic ply, which replaces the second mould part. In this connection, the dry fabric is placed in the mould, and air-proof covered by the plastic ply. In a next step, the air is evacuated from the whole set-up by a vacuum pump attached at the future outlet, thereby compressing the textile by the ambient pressure. Subsequently, an open resin reservoir is attached to the inlet, which, similar to the RTM process, establishes a pressure gradient and, in turn, initiates a resin flow from the inlet to the outlet. However, in contrast to the RTM process, the flexible plastic ply does not ensure the intended part geometry as the injection pressure, on the one hand, inflates the textile and, on the other hand, causes distortions in the alignment of the textile fibres. However, in order to allow for reliable predictions of the mechanical properties of the final structure, simulations of the overall manufacturing process are necessary.

The present contribution addresses the simulation of the resin flow process within the fibre fabric, where special attention is paid to the interaction between the resin and the deformable textile. The governing model proceeds from the Theory of Porous Media (TPM) [1], where the varying pore space is simultaneously occupied by a compressible pore gas, representing the ambient air, and an incompressible pore liquid, describing the resin. This approach allows for a continuous transition from the fully resin-saturated over the partially saturated, towards the fully unsaturated state, thereby accounting for the interactions between the pore fluids (resin and air) and the deformable fibre fabric. The governing equations are discretised and implemented into the finite-element-based research code PANDAS. However, in order to account for a straightforward application of the numerical model within a production-related environment, PANDAS is linked to the commercial FE package Abaqus via a general interface [2]. The capabilities of the presented modelling approach are numerically investigated in an element test, and the application possibilities are discussed in application-oriented large-scale parallel simulations.

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Yield stress fluid flows through porous media: breakage of the non-Newtonian character?

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ABSTRACT

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, original flow characteristics in through porous media may be expected. Here we discuss, both experimentally and theoretically the question of the Darcy's law (namely pressure vs mean velocity equation) for such fluids and the physical origin of its parameters.
The direct determination of this law is a challenge for several reasons: a non-linear relationship is expected, which implies that in order to determine it one has to make measurement in a wide range of velocities; usual techniques for determining the pressure may fail when applied to complex flows possibly exhibiting solid and liquid regions. Careful experiments nevertheless 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 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 [2] and as the pressure drop is increased more flowing paths progressively form within the porous medium. Such trends are in agreement with the flow characteristics through a single model pore. However, from measurements using a NMR technique (pulsed-gradient spin echo (PGSE)) not affected by spatial resolution problems, it was shown [3] that the velocity field of a yield stress fluid flowing through a disordered well-connected porous medium is very close to that for a Newtonian fluid. This result was confirmed by numerical simulation of 2D flow through disk packing [4]. 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 macroscopic regimes for flow of Carreau fluid in porous media

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ABSTRACT

The flow of generalized Newtonian fluids through porous media exhibit two asymptotic regimes that capture the dominant flow physics; Newtonian behavior at low Darcy velocities and power law behavior at high Darcy velocities. We consider Carreau fluid and develop an analytical model to predict the critical pressure gradient at which the transition from a Newtonian to a power law macroscopic behavior occurs. To validate the model, pore{scale simulations of shear thinning fluid flows in a 3D CT image of a sample of sandstone over a range of pressure drops are presented where the Carreau rheological model is used to estimate the fluid viscosity. These simulation results illustrate that the critical pressure gradient forecast by our model shows good agreement with the pore-scale simulations.

Estimating Permeability of Polyurethane (PU) Foams using 3D Micro-CT Images

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ABSTRACT

Polyurethane (PU) foams as cellular porous media have been used in different commercial applications because of their relatively high specific strength, low permeability, perfect insulating properties and high resistance to water absorption. In order to describe the suitability of a porous medium for flow-through applications, we consider different properties, but, among those, cell structure and permeability are often the most important ones. There have been a numerous studies on obtaining permeability as a function of cell size. Mills [1] applied computational fluid dynamics to determine the air-flow permeability for different types of open-celled polyurethane foams where the foam permeability was shown to be a function of the area of the largest hole in cell walls. From literature, it can be concluded that experimental determination or theoretical estimation of permeability using conventional or modified methods and models are limited by the type of foam under consideration, especially foams with different sized-holes on cell walls.
There has been some well-known models used to determine K for fluid flow through porous media; they are based on the mean particle diameter (D) and porosity (?) of the porous medium and have a general form, K= D2 f (?) [2]. These theoretical models do not take into account the cell connectivity during fluid flow through the foams. In porous media consisting of polyurethane foams, the small pores connecting the large cells face high pressure-drops during fluid flow. Therefore, it caused the measured permeability to be unusually low in polyurethane foam samples created in our lab. By using a micro CT-scanner, we obtained a 3-D image of our foam sample (Fig 1). The 3-D image was imported in COMSOL and the permeability obtained by simulating stokes flow through the pore space was 8.6e-11 m2. This value was found to be very close to the experimentally-measured permeability of 2.6e-11 m2 that was obtained using the falling-head permeameter. The theoretical permeability obtained using the standard permeability models was found to be around two-orders of magnitude higher. (For example, the Kozney-Carmen relation yielded a value of 77.8e-9 m2.) Hence, by using the 3-D image based flow simulation, we were able to account for the effect of higher pressure-drops in smaller inter-cell (hole) connections and obtain more reliable results close to the actual permeability.

Figure 1: A 3-D image of a polyurethane foam acquired using a micro CT imaging device

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A new methodology for effective, two-phase flow characterization of pore network structures

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ABSTRACT

The non-linear behaviour of two-phase flow in porous media, even in steady-state conditions is attributed to the interplay between capillarity and bulk viscosity. Capillarity regulates the flow for “relatively low” Ca values, whereas, for “relatively high” Ca values, the flow configuration is dictated -predominantly through saturation- by the bulk viscosities of the two phases. Since the actual independent variables of the process are the water capillary number, Ca, and the oil/water flowrate ratio, r, the flow configuration (capillary/viscous) depends on the flowrates of the two phases. The oil/water viscosity ratio, ?, regulates the flow range conditions for the transition from capillary to viscous dominated configurations.

A new methodology is proposed for the normative characterization of two-phase flows in porous media as capillary or viscous. Conceptually, it is based on the existence of a locus, r*(Ca), on which optimum operation flow conditions (OOC) are met and process operational efficiency [reduced flowrate of oil per kW dissipated within the system, f(Ca,r)], is maximized, Fig.1, [1,2,3]. In general, r*(Ca) is inversely proportional to Ca, and it can be approximated by a scaling function containing the oil/water viscosity ratio, ?, and two real, positive parameters A & B, eqn(1), Fig 2(a). The latter can be estimated from a set of laboratory determined optima for any particular oil-water-p.m. system. In addition, for any p.m. the various r*(Ca;?) corresponding to pairs of fluids with different viscosity ratios but same wetting, when appropriately scaled, collapse into a single function, R*(Ca), eqn(2), Fig.1(b).

I) Flow characterization. In any r*(Ca) or R*(Ca) diagram, the OOC locus plotted on a log-log scale, shows a significant mutation as Ca is increased from “small” to “large” values: the combined effect of viscosity and capillarity turns from capillary dominated to capillary/viscous to viscous dominated. A critical value of the capillary number, Cacv, segregating capillarity- from viscosity- dominated flows can be determined and detected at the maximum curvature of the OOC locus, 1/?.

II) Pore network characterization. The interplay between capillarity and viscosity, is expressed by the particular form of the normalized OOC locus described by values {A,B} associated with the particular pore network structure and wetting conditions. Therefore, in addition to flow characterization, the particular form of the normalized OOC locus can also be used to characterize the structure of a pore network. Parameters A & B, record the overall effect of the network structure across a variety of flow conditions /systems. Any locally maximum value of operational efficiency, depends on the total mechanical power dissipation that, in turn, depends on the structure of the porous network i.e. not only on absolute permeability, but also on tortuosity, pore size distributions and correlations, micro-roughness, fractal characteristics, heterogeneities etc. In this context, the pore network structure can be characterized by evaluating the indices A & B, universally representing its effect (“footprint”) on flow configurations spanning viscosity to capillarity dominated flow regimes. The proposed methodology is conceptually equivalent to mercury porosimetry.

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A Relation between Fractional Flow Rates in Immiscible Two-Phase Flow

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ABSTRACT

We present a set of equations that the fractional flow rates during two-phase flow must obey. These equations are derived from scaling symmetries that are obeyed under very weak conditions and they are closely related to thermodynamic relations such as the Gibbs-Duhem relation. We discuss how these equations give rise to relations between the relative permeabilities and capillary pressure. We compare our results with experimental data from the literature.

Validation of multi-phase lattice Boltzmann simulations for relative permeability prediction using process-based approaches

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ABSTRACT

The application of pore scale Digital Rock Physics methods to predict multi-phase flow parameters at the core and field scale is a great challenge. For this purpose, these methods have to be more thoroughly validated in direct comparison with experiments and theory. Here we describe the recent development of our lattice-Boltzmann method (LBM) simulation codes and present multi-phase flow validation results. For this purpose, we have implemented different multi-component models [1]. Here we will compare the effect of initial fluid distribution on hysteresis and relative permeability. First, we consider a random fluid redistribution in small steps, to allow for hysteresis effects. Second, we consider a new process-based relative permeability algorithm for the redistribution of the fluids. Third, we consider changing the pressure in the fluid phases as they propagate through the porous medium. The results from the new process-based models are compared with existing relative permeability calculation schemes, based on random initial distribution of the non-wetting phase, and available experimental data [2]. We observe good agreement regarding the steady-state relative permeabilities for both drainage and imbibition from our calculations in comparison with experimental data. Our numerical results demonstrate that the new relative permeability calculation schemes allow the consideration of hysteresis during the relative permeability calculation, which improves the accuracy of relative permeability prediction.

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Nonsteady-state Modelling of Deep Bed Filtration

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ABSTRACT

Deep bed filtration is an effective method of submicron and micron particle removal from the fluid stream. The quality of a filter can be described using three parameters, namely, pressure drop on the filter, its separation efficiency and retention capacity. They depend mainly on particle and filter pore size and material properties of particles and filter media. The presence of previously deposited particles produces the increase of both – filtration efficiency and pressure drop. It is worth noting that not only the total amount of deposited particles, but also their spatial distribution and structure affect filter performance [1]. Thus the development of a comprehensive model that takes into account all possible phenomena occurring during the filtration process is necessary.
In this work we have decided to examine the constricted tube model [2] for description of the filter structure. The overall structure of a porous medium is modeled as a cubic lattice of unit cells with constant inclination so as not to favor flow along any of the main directions (Fig. 1).
The fluid dynamics were modeled using lattice-Boltzmann approach . In this work 3-dimensional lattice with 19 allowed directions of movement (D3Q19).
Determination of structures of deposited particles on the filter fibre requires the knowledge of a history of the individual particle and its position and velocity vectors. The Lagrangian method of analysis [4] should be used for description of the process.
The aggregate motion model was developed by Moskal and Payatakes [5]. It assumes that the same forces that act on single particles act on aggregates. A simple approximate analytical expression was developed which estimates the drag force for each primary particle in an aggregate as a function of the number of its immediate neighbors. The translational and rotational motion of any aggregate of a given size, overall shape and internal structure is calculated through the numerical integration of a system of differential equations which describe the conservation laws of linear and angular momentum.
The resuspension model was described by Przekop et al. [6]. The Authors assumed that the adhesion and elastic reaction forces can be described by an equation of harmonic movement with dumping effect.
The models described above were used to simulate the deposition of spherical particles and aggregates in the system of constricted tube unit cells. Calculations were carried out for three different filters with the same thickness, 15mm, and porosity, 0.67, but with different pore sizes. The properties of the fluid and the particles were assumed to be the same as for water and SiO2, respectively. The superficial fluid velocity was assumed to be 2.5 mm/s. Figs. 2 and 3 show the time evolution of filtration efficiency and pressure drop of the filters, respectively. The calculations were carried until the pressure drop reached the value 5 times higher than the initial pressure drop. For the biggest solid particles we can observe a drop of the filtration efficiency at some stages of the process, which is caused by particle resuspension.

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Dynamic wettability alteration in immiscible two-phase flow in porous media

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ABSTRACT

When two immiscible fluids flow simultaneously through the same space, the capillary forces at the interfaces, the difference in the fluid viscosities, geometry of the medium and the wettability conditions make the flow properties extremely complex. Due to the vast range of applications in different areas like oil recovery, groundwater management, CO2 transport and storage and in catalyst supports used in automotive industry, the multiphase flow has been in the central attention of research since many decades. Here, we present a systematic computational study of how a continuous change in the wetting properties of the pores due to the flow of any wettability altering agent affects the partial flow of the fluids flowing through a porous media. This study has important implications in oil recovery where some 20 to 60 percent of the oil remains unrecovered in a reservoir after the production is declared unprofitable [1]. Wettability of reservoir pores can be altered by the injection of low salinity water and other wettability altering agents, and it is observed experimentally [2] and numerically [3] that the oil production increases when the pores are made more water-wet than oil-wet. However, the time-scale to increase the fractional-flow of oil during the wettability alteration is an important cost-related factor and it depends on the maximum possible change in the contact angle [4]. We model the porous medium by a network of disordered pores transporting two immiscible fluids. The instantaneous flow at the pore level obeys Washburn equation and the capillary forces are determined by a modified Young-Laplace equation. A time-dependent wettability altering mechanism is then introduced which simulates the continuous change in the contact angles at each pore, depending on the cumulative amount of brine passed through it. Simulations are performed to reach steady-states for different maximum possible change in the wetting angle (?). We find that deviation from oil-wet to water-wet conditions mobilizes the stuck clusters and increases the oil fractional flow. However, the rate of increase in the fractional flow with time depends strongly on ? and as ? ? 90°, a critical angle, the system shows a critical slowing down [5] characterized by two critical exponents.

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Counting of Configurational Microstates in Steady-State Two-Phase Flows in Continuous Pore Size Networks

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ABSTRACT

Steady-state two-phase flow in porous media is a steady-state, off equilibrium process -in the sense that it is maintained in dynamic equilibrium on the expense of energy supplied to the system. The efficiency of the process depends on its spontaneity, measurable by the rate of global entropy production. The latter has been proposed [1,2] to comprise two components: the rate of mechanical energy dissipation at constant temperature (a thermodynamic entropy component, Q/T, in the continuum mechanics scale) and a configurational entropy production component (a Boltzmann-type statistical-entropy component, klnW), that lurks within a discrete (and presumably countable) scale of flow microstates inherent in every flow configuration that is physically admissible with anyone, externally imposed, steady-state flow condition.
In a recent work [3], combinatorics have been implemented to evaluate the number of identified microstates per physically admissible internal flow arrangement that is compatible with the externally imposed flow conditions. The number of microstates, lnW, in steady-state two-phase flows in pore networks has been analytically derived in a closed form expression. The individual contributions of each prototype flow appear as Boltzmann-Gibbs type component expressions, implementing the volume fractions and size distribution of the various fluidic elements pertaining to the connected and disconnected interstitial oil flows.
In the present work, the previous analysis -pertaining to classes of pore sizes (of countable number) and classes of ganglion size- has been extended to account for continuous pore and ganglion size distributions.

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Integration of true-to-mechanism, flow-dependent relative permeability maps into FEM solvers for the investigation of transient, field-scale, 2-ph flows in porous media

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ABSTRACT

Most applications in the area of immiscible two-phase flow in porous media are based on inherently transient processes where one phase displaces the other, such as in drainage or imbibition. The combined effects of viscosity and capillarity (stemming from wetting and interfacial tension hysteresis effects as mobilized non-wetting phase is disconnected into fluidic elements of several sizes) is a key phenomenon regulating the relative permeability of oil and water in terms of the local flow conditions. These pore scale phenomena are efficiently handled and upscaled by the mechanistic model DeProF for immiscible steady-state two-phase flow in pore networks [1].
Extended simulations with the DeProF model algorithm in 3D model pore networks, delivered reduced macroscopic pressure gradient maps, x(Ca,r), as universal scaling law functions of the flow system independent variables, the capillary number, Ca, and the flowrate ratio, r, Fig.1, Eqs (1)-(3).
Such correlations were integrated within state-of-the-art FEM algorithms incorporating Darcian flow modules, in order to resolve field-scale transient flows in porous media for typical system configurations. The FEM solver considers the transient two-phase flow problem as an equivalent one-phase virtual flow with local effective mobility equal to the sum of the local phase mobilities. The algorithm solves the effective transport equation resulting from a combination of the Darcy law and the continuity equation for the virtual fluid, considering dependence of the effective permeability on local flow conditions. Mobilities and reduced pressure gradients are estimated from the DeProF permeability correlations, Eqs (1)-(2), for the corresponding field values. Saturation and superficial/seepage velocities for oil and water are then readily calculated from the virtual flow, provided the local values of Ca and r are available from the solution of the transport equation. The procedure is repeatedly integrated along sequential time steps.
The exponential form of the relative permeability correlations, Eqs (1)-(2), made the computational part of the problem extremely stiff, as the permeabilities may vary by orders of magnitude at locations near strong saturation gradients, such as drainage/imbibition fronts. In order to overcome the stiffness of the solution matrices, several preconditions were necessary to be applied in the solution procedure, including a sufficiently short time integration step.
The improved integration scheme has been applied to a variety of injection/production patterns. Indicatively, in a 13-spot well arrangement (regular 7-spot [2] with 6 additional wells, one at each side), oil in an initially fully saturated field is displaced by water, injected from the 12 adjacent wells at 350 MPa constant pressure, into the central extraction well. Figures 2a-d present consecutive snapshots (at 5, 10, 20 and 43 days) of the 1/12th of the 13-spot basic modular block. By modifying the initial configuration, the displacement of an oil plume can be predicted. Figures 3a-d present consecutive snapshots (at 0, 100, 400 and 750 hrs) of the oil plume displaced by water injected again at 350 MPa constant pressure.

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The statistical description of bubble flow in porous rocks

Presenter: Dick Bedeaux
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ABSTRACT

To study two-phase flow is quite relevant for the production of oil or water from boreholes. The flow occurs often in micro-meter-sized pores, which means that capillary effects are relevant. On the macroscopic scale, the average flow and the driving force (pressure difference) are most often related by Darcy's law. The proportionality constant, the permeability, depends on the relative amount of water in the material, the so-called water saturation, and the viscosities of the two fluids. A relevant question to ask is whether Darcy's law can be expected or predicted on theoretical grounds, given the two-phase nature of the flow, and the nature of the porous rock with non-negligible capillary forces.
A further question relates to the overall permeability and it relation to the partial permeability of the components.

In this work, we describe flow of the two immiscible fluids through a porous network of tubes, at the small and large scale, for one-, two- and three-dimensional cases using statistical thermodynamics. In particular, we are looking for a way to relate the permeability of the fluid components to properties of the porous medium. The small scale or local description is given for a tube in the model network; the global description aims to describe the average behavior of all connected tubes. In order to have a consistent description, the global one must follow by integrating the local one over the size of the system.

We have earlier seen [1] for the one-dimensional case, that the ensemble distribution is inversely proportional to the velocity of a bubble in the tube [1]. The ensemble distribution gives the probability that a bubble has a certain position in the tube, within the network. This observation allows us to develop a statistical mechanical description of the flow problem. For the 2- and 3- dimensional case we show that the property has general validity and that it holds irrespective of the number of bubbles in a tube. Analogous to the one-dimensional case we construct the ensemble distribution, which in addition to being inversely proportional to the velocity, now also describes the distribution of the flowing phases over the saturation and the radius of the tubes. We test the ensemble distribution using simulations of two-phase, steady-state flow in a random resistor network model, and find that indeed, it is inversely proportional to the velocity.

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Ultra-long time prediction of reactive solute transport in geologic formations using spatio-temporal upscaling: theory and numerical experiments

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ABSTRACT

Long-time predictions of reactive transport in porous media under time dependent boundary conditions and/or forcing factors require the formulation of continuum scale models for time-averages. Yet, as every macroscopic model, time-averaged models can loose predictivity and accuracy under certain conditions. This is true whenever lack of temporal and spatial scale separation occurs. In this work, we consider reactive transport of a solute undergoing a heterogeneous reaction and subject to time-varying boundary conditions in a periodic porous medium. By means of homogenization method, we derive macro-time continuum-scale equations and show i) that the dynamics at the macro-scale (Darcy-scale) is strongly influenced by the interplay between signal frequency at the boundary and transport processes at the pore level and ii) under which conditions space-time averaged equations accurately describe pore-scale processes. Finally, we test our theoretical results through numerical simulations of transport in a planar fracture with reacting walls and time-varying boundary conditions at the inlet. Our analysis shows a good match between numerical simulations and theoretical predictions.

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Modeling porous media hydrodynamics at different spatial scales

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ABSTRACT

Spatial averaging over a Representative Elementary Volume (REV) of intensive quantities product leads to concurrent PDE's, describing macroscopic balance equations of the phase extensive quantity at the REV spatial scale and the one associated with the deviation from that extensive quantity at a much smaller scale.
The hydrodynamic characteristics at the smaller scale are governed by pure hyperbolic PDE's (Sorek et al., 2005; Sorek et al., 2010; Sorek and Ohana, 2015). Field observations of condensed colloidal parcels motion (Ronen et al., 1992) under natural gradient flow validate the suggestion of hyperbolic PDE's addressing the fluid momentum and components mass balance at the smaller spatial scale.
At the REV scale, Sorek et al. (2005) obtain extended forms of the macroscopic Navier-Stokes (NS) equation. These can vary from inertia fluxes in the form of a nonlinear wave equation, Forchheimer's law expressing the microscopic NS fluid inertia transmitted to the solid matrix through the solid-fluid interface (Sorek et al., 1992; Levy et al., 1995, Levy et al., 1999), or conform to Darcy's law when friction at that interface is dominant.
Controlled experiments supplemented by numerical predication of the primary and secondary macroscopic balance PDEs are needed to study the hydrodynamic interrelation between these two adjacent spatial scales.

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Gas slip-flow in homogeneous porous media: the macro-scale model revisited

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ABSTRACT

In this work, the macroscopic model of isothermal, slightly compressible, gas slip-flow in rigid homogeneous porous media is revisited by upscaling the microscopic mass and momentum equations with a first-order slip boundary condition at the solid-fluid interface [1-3] corresponding to a small enough Knudsen number (up to Kn=O(0.1)). The method of volume averaging is employed leading to a Darcy-like model in which the apparent permeability, Ks, is determined by solving a non-intrinsic closure problem, that is Kn dependent. It is observed that, under some circumstances, Ks depends non linearly on Kn.
A further development is carried out relying on an expansion in the Knudsen number. With this procedure, the model is such that Ks is decomposed under a series of tensorial effective quantities, all of them being determined by solving intrinsic closure problems which are coupled at the successive orders in the macroscopic Knudsen number. At the zeroeth order, the model reduces to the classical Darcy's law while the first order yields the classical slip correction, linear in the Knudsen number considered so far in the literature [4]. The corrective terms at the higher orders are shown to be non negligible in some cases and contain the non linearity in the Knudsen number observed on Ks.

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Two-Phase flow in porous media at high Reynolds number: discussion of macro-scale models based on new experimental data

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ABSTRACT

A new experimental device set-up has been developed at IRSN to measure pressure drop, phase velocities and average saturation over a porous column subjected to a high Reynolds water-gas flow. Experiments were realized for various water and gas velocities typical of situations encountered in nuclear safety problems. The results are interpreted in terms of average saturation as a function of the velocities, and pressure drop as a function of average saturation and velocities.
These experimental data are used to discuss the potentially acceptable macro-scale models as well as the probable form of non-linear effective parameters. In particular it is shown that classical generalized Darcy's law lack the necessary features to model the pressure drop. Model with cross terms on the contrary may be used to reproduce experimental data.

Digital Rock Physics: Comparison between carbonate reservoir rock and standard dolomite rock

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ABSTRACT

The emerging field of Digital Rock Physics (DRP) makes use of advances in imaging technology and computational power to generate flow properties. This allows for a variety of studies to be conducted on the same imaged dataset without compromising the sample. While standard core plug experiments allow for the determination of properties such as permeability in a single direction, the versatility of digital rock physics allows for studies to be done in all three directions. Properties such as anisotropy and heterogeneity may thus be investigated. This opens the doors to better characterize core plugs and leads to better analysis and modeling of hydrodynamic phenomenon at the pore scale. Upscaling this knowledge from the pore scale to the reservoir scale is important for geotechnical studies in the fields of oil and gas as well as carbon capture.
In this work, we digitally compare the physical properties of two different core plugs; one from a carbonate reservoir and the other a standard dolomite sample. The workflow starts with the volume reconstruction of microCT images of 1.5 inch samples. These images are segmented to separate the void from the solid matrix. Then numerical simulations are conducted to determine the property-dependent representative volume element with a focus on porosity and permeability. Simulations are conducted using the open-source software Palabos that runs a Lattice Boltzmann algorithm as well as the Avizo Absolute Permeability Plug-in that solves the Stokes' equation directly using the Finite Volume method. In the analysis we focus on evaluating how the difference of isotropy and homogeneity in the samples affect the validity of the workflow. We also compare the computational results of both numerical methodologies on both types of samples.

Two phase inertial flow in model porous media: a numerical investigation

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ABSTRACT

The two phase inertial flow in porous media, characterized by Reynolds numbers larger than the unity, is encountered in many industrial applications such as flow around wells in oil recovery and flow in column reactors for chemical engineering, etc. Due to the difficulties related to its treatment, the bibliography related to this kind of flows remains poor. This work tackles some important aspects of two phase inertial (stationary) flow of Newtonian incompressible and immiscible fluids in an ordered square lattice of cylinders of circular cross section (see fig. 1), the wetting and non-wetting fluid phases being distributed under the form of continuous channels. The analysis relies on the macroscopic model derived elsewhere and resulting from the upscaling procedure applied to the microscopic balance equations and boundary conditions [1]. The effective properties (dominant and coupling permeabilities; dominant and coupling inertial corrections) appearing in the macroscopic model are determined from the resolution of the microscopic flow and the associated closure problems. We first show here that the coupling permeabilities, that are generally neglected in the generalized Darcy's law [2], can be, in certain configurations, of the same order of magnitude as the dominant permeabilities and therefore cannot be ignored. The same observation can be made for coupling inertial corrections that are close to the dominant ones. It is also shown that the inertial correction may exhibit, in some situations as that considered here, a quadratic dependence upon the Reynolds number (cubic dependence upon the filtration velocity), unlike the classical Forchheimer correction type (quadratic dependence upon the filtration velocity) as assumed in the empirical Darcy Forchheimer model [3,4]. Finally, it is observed that, whereas inertia opposes a resistance to the flow in the wetting phase, it tends to enhance flow in the non wetting phase due to a mechanism that can be interpreted as a lubrication phenomenon as shown in fig. 2.

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Upscaling binary gas dispersion under slip conditions

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ABSTRACT

Modeling of gas dispersion in porous media is of interest in many applications ranging from nanofluidic systems to subsurface contaminant transport. In this work, we derive a macroscopic model to study slightly compressible binary gas dispersion in homogeneous rigid porous media for conditions in which the tangential fluid velocity undergoes a slip at the solid interface due to Knudsen effects and to mass diffusion. The method of volume averaging is employed to derive the governing equations at the Darcy scale for both mass and momentum transport. The momentum transport model consists in a modified Darcy's law which includes a correction due to Knudsen effects and a additional dispersive term due to diffusive slip. For mass transport, the resulting model is the conventional convection-dispersion equation with two correction terms, one affecting convective transport and the second one affecting mass dispersion due to gas compressibility. The macroscopic model reduces to the one reported by Altevogt et al. (2003) for the case in which gas slip is only due to a concentration gradient and to the one by Lasseux et al. (2014) when slip restricts to Knudesn effects only. The model is written in terms of effective-medium coefficients that can be predicted from solving the associated closure problems in representative unit cells. When Knudsen slip is thought to be dominant compared to diffusive slip, our computations on some model 2D porous structures indicate that the predictions of the longitudinal dispersion may differ by 20% compared to the predictions obtained by ignoring gas slip.

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A Polarizable Force Field to Study Cations and Water Molecules Dynamics in Montmorillonites

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ABSTRACT

The wide use of clay minerals in industrial applications (catalysis, formulation), energy and ecological engineering (oil recovery, ground water remediation, geological barrier for radioactive waste and CO2) is partly due to their remarkable properties of retention at the mineral surface. In environmental engineering, the role of water on clay permeability and retention properties is crucial. Indeed, the water is the vector of the motion of the species present in the medium, hazardous elements for instance.
Clays are lamellar inorganic materials composed of layers piled on top of each other to form particles. Clays show different behaviors towards water, depending on the value of the negative structural charge carried by the mineral layers: although hydrophobic when uncharged, a clay can become hydrophilic when charged. In particular, clays swell or not, depending on the hydration property of the counter-ions located between the layers.
Molecular simulations allow a detailed picture of the structure, thermodynamics and dynamics of the fluid at the interface. They are already used to explain the hydrophobic/hydrophilic property of various clays such as : Talc, Pyrophyllite and Montmorillonite[1,2]. Unfortunately, the numerical results do not always reproduce quantitatively the experimental results, which casts, consequently, a doubt on the validity of simulations interpretations[3]. In particular, the polarizability, which is not taken into account could play a significant role especially when an electric field is present at the interface[4] .
Therefore, we developed a polarizable force field based on DFT calculations. The dry structures of montmorillonites with different types of counter-ions (Na+, Cs+, Ca2+ and Sr2+) are simulated and compared with X-ray experimental data. Then, the polarizable force field is used to study the diffusion of cations and water molecules in montmorillonites. Our results are compared with the results obtained with the non polarizable force-fields ClayFF and with the available experimental data.

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Scanning SAXS-WAXS microscopy applied to shales to bridge the pore and macroscopic scale

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ABSTRACT

The pore sizes in shales typically range from molecular dimensions to micrometer in size changing their characteristics on an even larger scale. The huge variation of length scales is a challenge for the determination of the microscopic rock fabric of shale rocks. While standard characterization techniques generally provide volume averaged properties of the pore network, high resolution imaging techniques do not assess representative regions of interest. Due to this dilemma open questions remain regarding the role of the pore network extending over multiple scales for retention and transport processes, e.g. during production. In this contribution, volume averaged but localised information about the meso and micro pores (1-100 nm) is obtained applying scanning small- and wide-angle X-ray scattering (SAXS and WAXS) microscopy1,2. SAXS-WAXS pattern are collected in a raster scanning microscopy mode, such that micrometer sized volumes are collected over a (2 x 2) mm2 large scanning area. Thus, simultaneously from the local assessment porosity, pore size distribution and orientation, as well as mineralogy can be derived. Aiming at a full characterization of the shale pore network, the measurements and subsequent matrix porosity analysis are integrated in a multi-scale imaging workflow involving SEM/EDX and ?CT analysis. The length scale ranges covered are nm to millimeters, leaving a gap that possibly can be closed in future work.

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A New Coupled Discrete Fracture-Reiterated Homogenization Approach for Modeling Flow in Shale Gas Reservoirs

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ABSTRACT

A new multiscale model for coupling gas flow in hydraulic fractures and multiporosity shale matrix is constructed within the framework of the homogenization procedure in conjunction with the discrete fracture modeling.
For the hydrodynamics in the shale matrix we construct a new pressure equation where the shale is envisioned an homogenized matrix composed of interparticle pores and nanopores within the kerogen along with an impermeable inorganic matter. The pressure equation is coupled by source terms with the governing equations for single phase compressible flow in the hydraulic fracture network. An extended variational formulation contanining the hydrodynamics of the two systems occupying distinct domains is constructed and discretized by the finite element method giving rise to a discrete fracture multiscale approach for unconventional reservoirs. The resultant system is capable of capturing the behavior of the gas in the nano pores and upscaling and coupling with flow in a random arrangement of hydraulic fractures. Numerical simulation of gas withdrawal are presented illustrating the potential of the formulation in computing with accuracy gas production curves

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Exploring multi-phase flow phenomena of fine-grained reservoir rocks: insights from ethane permeability measurements

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ABSTRACT

The multi-phase flow phenomena of fine-grained reservoir rocks are important for modelling and predicting hydrocarbon production from shale gas and shale oil reservoirs. However, these phenomena remain underexplored in the laboratory due to difficulties associated with controlling and determining fluid saturation in nano- to micro-Darcy permeability rocks. In this study, multi-phase flow phenomena of a suite of fine grained sedimentary rocks were investigated by measuring permeability to gaseous ethane over a range of pore pressures from 0.7 to 3.4 MPa. Ethane was chosen as a probing gas because the saturated vapour pressure of ethane is within easily reached laboratory pressure-temperature conditions. Saturation of liquid ethane increased due to adsorption and capillary condensation as pore pressure approached the saturated vapour pressure of ethane at the temperature of the permeability measurements (3.7 MPa at 293 K). Although the gaseous ethane-liquid ethane fluid system is not a typical fluid system of interest for hydrocarbon reservoirs, the data in this study are relevant as other laboratory data pertaining to this important topic are sparse.
For all rocks, permeability to gaseous ethane decreased with increasing pore pressure. Permeability at 3.4 MPa was up to 1.5 orders of magnitude lower than permeability at 0.7 MPa. Between 0.7 and 1.4 MPa, permeability decayed with pore pressure in a way that would be expected due to gas slippage, as inferred from gas slippage measurements made using helium as a probing gas. Between 1.4 and 3.4 MPa, permeability to gaseous ethane decayed by too much to be explained by gas slippage, and was therefore interpreted to be the result of increasing liquid ethane saturation. Ethane isotherms were collected and used to estimate the saturation of liquid ethane over the pressure range of the permeability measurements. Hysteresis loops were observed when permeability was measured with both increasing and decreasing pore pressure. The hysteresis loops show the opposite behaviour of what would be expected due to capillary condensation in mesopores, and these loops remain under study.

Diffusion under extreme confinement: finite-size effects in molecular simulation.

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ABSTRACT

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), which 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. We will discuss the finite-size effects in all directions, for model systems (LJ) and more complex ones (water between clay layers). We will propose an analytical model to determine the effect of finite-size on diffusion coefficient according to the box size.

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LOW PERMEABILITY MEASUREMENTS ON SMALL ROCK SAMPLES

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ABSTRACT

This paper describes an original method for measuring very low permeabilities on small rock samples. Rock size ranges from 0.5 to 2 cm, and at atmospheric pressure, the lower limit of measurement is close to 0.1 nanoDarcy.

A small rock sample (under 1 cm3) is first embedded in a resin and a 2 to 5 mm thick disc is cut, polished, and placed in a core holder under vertical confining stress. The gas permeability is derived from measurements of pressure or flow rate, similar to a standard plug. The equipment operates with upstream pore pressures ranging from vacuum to 10 bar (which could be increased). The outlet pressure remains close to atmospheric pressure. A numerical calculation is developed taking into account Klinkenberg effect with automatic history matching. This equipment has been tested on shales and other rock samples with a large range of permeabilities (nanoDarcy and microDarcy range).

For gas permeabilities larger than 10 nanoDarcy (at atmospheric pressure), both permeability and Klinkenberg coefficient are derived by numerical history matching either from a single pressure decay experiment, or several measurements at different pressures, similar to commercial equipment.

For very low permeabilities (below 10 nanoDarcy at atmospheric pressure), leaks in the upstream portion of the equipment are no longer negligible and the production needs to be measured at the outlet. Permeability is then derived from the increase in pressure in a small volume at the outlet. The pressure remains very close to atmospheric pressure, and a reference measurement compensates for variations in atmospheric pressure and temperature. This method is much more accurate than any commercial flowmeter.

During a measurement, the outlet pressure does not start to increase immediately after setting the inlet pressure. The delay in production is due to gas compressibility and is a function of the sample porosity. For the lowest permeabilities, the delay can be of several hours before a linear increase in pressure can be obtained. Importantly this delay is used as a quality control: it allows a verification of the measured porosity, and when the sample is fractured or leakage is present, there is no delay and the measurement is discarded.

With this method, the lower limit for gas permeability is approximately 0.1 nanoDarcy at atmospheric pressure, resulting in gas permeabilities of 1 picoDarcy at 100 bar. In this domain, the Klinkenberg term b/P is much larger than unity, and the liquid permeability cannot be determined (the Klinkenberg line passes through the origin). Experiments performed at different pore pressures confirm the linear behavior with 1/P.

One advantage of this method is that analysis can be performed on small pieces of rocks of irregular shape when large cylindrical plugs are not available. Another advantage compared to plugs is the relatively short duration of measurements. For the lower limit of gas permeability (0.1 nanoDarcy), with a disk thickness of 5 mm the duration of the delay is around 10 hours. For a 5 cm plug, the duration, which is a function of the length squared, would be 40 days!

The effect of wettability and soak time on hydraulic fracturing with lattice Boltzmann method in tight reservoirs

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ABSTRACT

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 recovery of fracturing fluid during hydraulic fracturing is much lower than that in conventional reservoirs. “The fraction of the volume of injected water that is recovered as flowback water from horizontal wells in Pennsylvania ranges from 9 to 53%, with an average of 10%. It has been observed that the recovery can be even lower than 10% if the well is shut-in for a period of time.” is reported recently [1]. For tight oil in Changqing oilfield, meanwhile, the production with shut-in for soaking after fracturing is better than that without this process. It is considered that the reservoir rocks contain huge number of micro-pores, and the oil (as nonwetting phase) in micro-pores is replaced into micro-fractures by fracturing fluid (as wetting phase) under capillary force.

In this study, simple channel model is designed at first, and the replacement phenomenon is confirmed by lattice Boltzmann simulation. Beyond that, the replacing condition is studied. Then three back to back processes in hydraulic fracturing, which are fracturing fluid injection, shut-in for soaking, flowback of fracturing fluid, are simulated in a pore network model constructed with different size pores and throats. During the simulation, different wettability and soak time are given and their effects on hydraulic fracturing are studied.

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Fluid transport through the porous media with irregular distribution of heterogeneities

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ABSTRACT

In this work we consider fluid (shale gas) transport through the heterogeneous solid having complex structure of pores. Heterogenieties are imbedded into a uniform matrix. There exist a contrast of properties and spatial scales between the matrix and inclusions. The pore size can vary from micro- to nanometers, permeability and diffusivity can differ by several orders of magnitude. We present an approach, which allow us to apply upscaling techniques to the case of irregular distribution of heterogeneities. We focus on the upscaling from pore-scale to the core-scale and then from core-scale to reservoir scale. It turns out that macroscale parameters characterizing fluid flow are based on pore-scale simulations As a result of upscaling we obtain homogenized macroscopic equations with effective coefficients. These coefficients depend not only on the spatial structure of the medium and properties of both inclusions and matrix, but also from some parameter ?, which characterizes the average deviation from the regular (periodic) distribution of heterogeneities. We investigate the sensitivity of effective characteristics to different values of diffusivity, permeability and porosity of the matrix and inclusions as well as to the variations of the value of parameter ?. We solve macroscopic problem and determine the distribution of fluid concentration in effective medium for the given initial and boundary conditions.

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Multiscale Simulation of Gas Flow in Shale Formations

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ABSTRACT

Shale gas reservoirs have become major sources of natural gas production in North America, and are expected to play an increasingly important role in Asia in the near future. Over the past decades, advanced techniques such as horizontal drilling and multi-stage hydraulic fracturing have greatly promoted the exploitation of shale gas from low permeability reservoirs. It is widely agreed that with hydraulic fracturing the fabric of shale systems comprises primarily organic matter, inorganic minerals, natural fractures, and hydraulic fractures. Multiscale porous structures coexist in shale gas reservoirs, with totally different characteristics with regard to porosity, permeability, wettability, gas storage, and flow mechanisms. Further, multiple physicochemical processes simultaneously take place within the multiscale porous systems including surface diffusion, desorption, Knudsen diffusion, viscous flow, particle flow, etc. Modeling such complex transport processes remains a grand challenge due to the inherent heterogeneity of shale formations and uncertainties associated with their characterization, as well as the difficulties in conceptualizing and describing fluid flow and mass transport processes in such a complex system.

We have developed a multiscale simulation strategy by adopting numerical methods at different scales including molecular dynamics method (MD), the lattice Boltzmann method (LBM), and reservoir simulators. First, adsorption phenomenon on the surface of inorganic and organic matter of nanosize pores was simulated using the MD. Effects of pressure, pore size and solid wall affinity on the thickness of adsorption layer were investigated. Second, Knudsen diffusion and viscous flow in organic matter and inorganic matter with fully resolved micro/nano-scale pore structures were studied using the LBM. Apparent permeability was calculated using the Dusty Gas Model based on effective Knudsen diffusivity and intrinsic permeability predicted by the LBM, and was compared with that determined with empirical correlations such as Klinkenberg's correction and Beskok and Karniadakis-Civan's correlation. Third, a generalized LB model was developed for REV-scale shale matrix. Effects of mineral content, mineral distribution, grain size, inter-particle pores, adsorption, and slip flow on the REV-scale shale matrix permeability were explored. The generalized LB model was also applied to matrix-fracture systems and a power-law relationship between the fracture density and effective permeability was revealed. Finally, surface diffusion of adsorbed gas was considered using the generalized Maxwell-Stefan model (GMS), and its effect on the effective permeability of the shale matrix was studied using the generalized LB model.

Pore Space Superposition Reconstruction Method for Shale Samples

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ABSTRACT

A shale matrix is too tight to be described using conventional methods, and digital core technology is becoming an alternative method. Because both organic and inorganic pores exist in the shale matrix, a digital core and a pore network model that could describe these two types of pores at the same time are constructed in this paper. Firstly, the inorganic pore digital core is constructed based on the multiple-point statistics method, and the organic pore digital core is constructed based on the Markov chain Monte Carlo method. The two types of digital cores are superposed together according to a superposition algorithm, which includes information about the shale organic and inorganic pores. The pore network models of different constructed digital cores are extracted using the pore space medial axis method. Finally, based on these platforms, the geometry and topology structure properties, the pore size distribution and the coordination number of a shale sample are analyzed. The results show that the pore size distribution of the shale sample generally ranges from 2 nm to 100 nm, mainly distributing from 5 nm to 20 nm. The coordination number is almost always in the range of 2 to 3. The digital core results match well with the experimental results to some extent for our study case.

A multiscale pore network modeling of gas flow in the nano-porous media of shale

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ABSTRACT

1. Objectives
Shale is characterized as an ultra-tight porous media with pore size mainly distributed in the range of nanometers. In these nano-pores, mean free path of gas molecules is typically comparable to the size of nano-pores and gas-wall collisions become significant. The continuum assumption breaks down and effects of compressibility and rarefaction are present. Consequently, non-continuum flow regimes, including slip flow, transition flow and free molecular flow, are encountered in the nano-porous media. Currently both numerical and analytical methods have been developed to study the gas flow in 2D (Sakhaee-Pour and Bryant 2012) and 3D porous structures (Chen et al. 2015) of shale. Although improvements have been gained, they fail to detail the flow behavior (such as rarefaction effect and slip velocity along the pore walls) in the nano-porous structure of shales. In order to improve current studies, we present an innovative methodology in the present study to simulate gas flow in a representative pore network of shale by employing a kinetic-originated method – the extended lattice Boltzmann method (LBM).
2. Methods and Procedures
In this study, the porous structure of a shale matrix (1?m×1?m×2?m) is characterized by FIB/SEM images and represented by a 3D pore network model. Flow simulation is then carried out in following steps. Firstly, rarefaction effect of gas flow in a single channel is simulated by the extended LBM. The obtained velocity profile and flow rate are validated with solution of linearized Boltzmann equation and direct simulation Monte Carlo. Based on LBM simulation, a correction factor, which correlates the equivalent gas permeability of non-continuum flow with intrinsic permeability of continuum flow, is derived to extend the application of Darcy equation to the non-continuum regimes. This modified Darcy equation is then employed in the pore network to simulate the dynamic flow processes and estimate gas permeability. Sensitivity analyses are lastly carried out to test the effects of pore size distribution, pore connectivity and reservoir conditions on the apparent permeability of the nano-porous media.
3. Results
Pore network of the shale matrix is reconstructed on the basis of FIB/SEM images with resolution down to 4 nm. Physics of rarefied gas in the confined space are well captured by the extended LBM and simulation results are up-scaled to the pore network. Results show that the flow rate is mainly contributed from slip flow and transition flow. The slip velocity in the rarefied flow contributes extra flow rate and results in a higher apparent permeability. Sensitivity analyses also show that the contribution of transition flow becomes prominent when the fraction of nano-pores increases and/ or reservoir pressure declines.
4. Novelty
This study presents a novel technique to simulate the complex flow processes in multi-scales (single capillary and pore network) in shale. The innovative image reconstruction and flow simulation allow us to model the flow behavior in nano-porous media accurately and efficiently, which provides a basis for new generation of reservoir simulators.

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An approach for characterizing the apparent permeability of organic-rich shale oil reservoirs

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ABSTRACT

The shale matrix consists of multiple continua with organic and inorganic pores that adds the complexity and unpredictability to measure the permeability of an organic-rich shale oil sample. The complexity and unpredictability are mainly caused by the various laboratory conditions, the fluid-storage and transport mechanisms in shale matrix. Especially, the solid/liquid interactions in organic-rich shale are larger in comparison to the natural gas, which has significant effects on the permeability and the production. However, there is still not a comprehensive apparent permeability model considering the multiple transport mechanisms in shale oil reservoirs.

In this study, various transport mechanisms are considered in organic and inorganic matters respectively. The single-phase liquid hydrocarbons flow in nanoscale organic cylinder-shaped pores can be described by the Darcy's law and the Brunauer-Emmett-Teller equation which is a typical characterization for multilayer adsorption, whereas the molecular slippage on the inorganic-pore walls is introduced to make the liquid flow in nanoscale inorganic cylinder-shaped pores properly. Combining with different transport properties such as intrinsic permeability, tortuosity and porosity, an approach to characterize the apparent permeability of organic-rich shale oil reservoirs is developed that couples the adsorption effect in organic pores with the molecular slippage in inorganic pores. The calculated results show that the presented permeability model provides a better prediction of oil production by pressure driven force.

The effects of parameters on the intrinsic and apparent permeability are presented including the mean pore radius, pore pressure, friction coefficient, tortuosity, porosity, slip length and the adsorption. The transport properties relevant to the nanoscale porous medium influence on both the intrinsic and apparent permeability, while the slip phenomenon and adsorption can cause the significant difference in apparent permeability. Slip phenomenon of liquid flow in nanoscale inorganic pores leads to the apparent permeability larger than the intrinsic one. On the other hand, the sorbed phase make a portion of hydrocarbons unrecoverable in smaller nanoscale organic pores.

Hence, the characterization of the apparent permeability of organic-rich shale oil reservoirs is important for estimating the oil-in-place, predicting a well performance and its oil production.

Modeling of multi-scale flow in ultra-tight shale oil reservoir

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ABSTRACT

This paper present a new approach to characterize nanopore structure and its multiscale feature in shale oil reservoir. Unconventional shale reservoir are very low permeability and strongly heterogeneity caused by various scales of nanometer- to mircrometer-size pores and conglomerations of organic matter. The heterogeneity of the microscopic structures have significantly affect the shale permeability and larger-scale transport properties. It has been shown that the slippage phenomenon is very common between liquid and boundary interface in micro- and nanoscale fluid flow, slip length could range from few nanometers to hundreds of micrometers. The apparent liquid permeability increases due to average pore radius of shale strata decreases. However, single nano-sized tube is limited to characterize multiscale flow within multiscale pore space. In practice, this paper provides an efficient and simple model to quantify the flow and transport in complex multiscale heterogeneous media. In this paper, we formulate a scale-dependent permeability function, referred to as the apparent permeability model, assuming that liquid slippage are the main contributors to the overall flow in porous media. To account for the number in any pore-size space and tortuosity of pore network, we introduced fractal theory to describe multiscale pore structure. We also considered corresponding flow behaviors and properties within a specific pore-size interval. The results shows that multiscale flow have significant impact on liquid rich shale permeability. This model provides a novel and efficient approach to describe impact of multiscale flow behavior.

The mesoscopic mechanism of in situ thermal exploitation oil and gas of oil shale deposit and THMC coupling numerical simulation

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ABSTRACT

oil Shale deposit is huge reserves, and undeveloped important unconventional oil and gas resources, scholars in many countries around the world are committed to in situ distillation of oil shale, as not yet the development of industrial scale. Authors devotes to the in situ thermal oil shale mining research for more than 20 years, this paper introduces under the action of different anaerobic dry distillation temperature, microscopic CT technology for oil shale pore, the changing rule of the microcracks, expounds the change of microscopic pore and fracture in situ heating oil shale, relevant laws and the dry distillation and oil and gas migration. Put forward of coupling mathematical model for deformation, seepage, heat and mass transfer in situ thermal oil shale mining shale oil? and with a large number of numerical simulation studies, revealed to process and law of heat transfer and pyrolysis from the macroscopic fracture to micro crack and pore, provides scientific guidance to thermal exploitation in situ of oil shale.

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Multi-scale core to pore imaging and modelling of the Rotleigend Sandstone

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ABSTRACT

Geologic systems are heterogenous on all length scales1. Reservoir engineering captures such heterogeneity by classifying the formation into multiple lithological facies, constructing reservoir models and sampling these for further examination using core analysis. This process, however, only captures heterogeneity down to the scale of the 1 – 1.5” “core plug”, which is then upscaled back to the reservoir model.

Over the last 15 years pore scale imaging has developed from an academic tool for the investigation of fundamental displacement processes to an increasingly utilized industrial technique for the characterization of systems down the nm level2. While much progress has been made3,4, significant challenges remain, including that of scale and heterogeneity. Frequently pore-scale imaging can achieve the 3D resolution required to capture the pore structure of a wide range of rock types only by sacrificing a field of view sufficient to capture macroscopic heterogeneity. Recent developments in imaging technology can be used to bridge the gap between pore and reservoir-core scale descriptions. As imaging and analytical technology has developed, boundaries between different imaging technologies have become less distinct, and for the first time there is an integrated capability for 3D imaging spanning length scales all the way from 4” whole core down to the nm.

This paper presents a novel methodology for classifying, sampling and imaging a 1” core-plug such that essential heterogeneity is maintained throughout the workflow. This is applied to a subsurface sample from the Rotleigend sandstone, a central European reservoir showing strong lamination on the mm-cm scale. First the entire core-plug sample was imaged with a resolution of around 19µm. While the pore structure was not resolvable, macroscopic bedding related heterogeneity was, along with a prominent fracture. This image was classified, creating a label image where each voxel was either labelled as a “high porosity”, “low porosity” or fracture. Locations for high resolution (1-3µm) non-destructive interior tomographies were defined using this macroscopic lithological map. As mechanical sample extraction was not required, sample sites could be much more accurately identified, and the association between litho-type and microscopic structure maintained.

Permeability tensors were calculated for each interior image. A second model was then constructed using the macroscopically classified image, so each voxel from the high porosity and low porosity lithologies were populated with the associated average permeability tensor derived from the high resolution images. A simulation was then performed, computing stokes flow through the macroscopically visible fracture and Darcy flow through the microscopically sampled lithologies. The resulting permeability tensor was highly anisotropic, with a high permeability in directions parallel to layering and low permeabilities perpendicular to it. This result was only possible because the cm scale heterogeneity associated with primary sedimentary layering was maintained, through the macroscopic model.

While this method has been applied specifically to permeability calculation, it can be viewed as a

general framework for dealing with heterogenous multi-scale systems, both for volume averaged properties (e.g. porosity & total organic content), directional properties (e.g. permeability & formation factor) and even complex multiphase properties (e.g. relative permeability & transport effects).

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Micro-nano Scales Flowing Simulation in Shale Gas

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ABSTRACT

The storage space of shale reservoir is mainly composed of complicated nanoscale pore, in which the gas exists in the form of absorbed gas and free gas. Due to the complicated pore structure and various gas storage states, gas flowing in the pore space is affected by multiple transport mechanisms including adsorption, desorption, Darcy flow, slippage and diffusion, etc. Therefore, a comprehensive research on the effects of transport mechanisms on shale gas flow is the key to study the shale gas migration rule, evaluate production capacity, and make reasonable development plan. Firstly, according to the physical meanings and interactive relationships of transport mechanisms, the flowing mathematical model is established for the pure methane gas. Then, based on the pore network model, which takes both the geometrical morphology and topological structure of shale matrix pore space into consideration, the above flowing mathematical model is discretized to construct the corresponding pore network flowing numerical model. Finally, gas flowing simulation is carried out by solving the model. The impacts of various transport mechanisms on gas flowing in the process of shale gas development under different physical properties and pore pressures are studied, and the changes of gas flow mechanisms at different stages are also analyzed. The research results will contribute to the understanding of the gas transport rules in shale gas reservoir, improve seepage theory of this unconventional reservoir and provide a theoretical support for rational development plans.

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Simulation of elastic deformations with damage effects for porous rocks under external and pore pressure

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ABSTRACT

The microstructure of porous rock samples from drill cores can be characterized by µCT images of high resolution.
In this paper such imaged rock samples are taken as computational domain to simulate both the mechanical deformation due to internal pore pressure and due to external compressive loads on the outer surface of the sample.
The resulting local mechanical stresses may lead to the growth of microcracks which are approximated effectively by a continuum damage model. Then a local permeability is introduced as a function of the damage variable. Finally, we show, how the fluid flow through the sample depends on the magnitude of the compressive load, i.e., on the evolution of the damaged zones.
The considered periodic boundary value problem in nonlinear elasticity is discretized on a regular grid (voxel grid) and solved by using a FFT-based iterative scheme.
Numerical tests are presented to demonstrate the dependency of the effective macroscopic permeability from the compressive loads. The parallelization and numerical effort for resolutions up to 1024x1024x1024 voxels is discussed.

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Influence of Pore Structure Parameters on Flow Characteristics based on a Digital Rock and the Pore Network Model

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ABSTRACT

Many approaches have been developed to study the role that pore structure parameters play in flow characteristics. In this paper, 2D regular models are used to study the influence of the porosity, particle size, pore throat opening, pore throat ratio, coordination number and shape factor on the absolute permeability; the pore network model is adopted to analyze the relative permeability curve with a changing coordination number and shape factor; and a digital core, based on CT scanning, is constructed to study the relationship between the flow limit and the pore structure that determines whether the fluid can flow at a certain pressure. Because the scale of a pore is much larger than the average free path of the molecules that travel through the pore, the fluid in porous media can be seen as a continuous medium, and its flow characteristics are in line with the classical hydrodynamic theory. To accurately describe the fluid flow in models, the Navier-Stokes equation (N-S equation) is selected to control fluid motion in this paper; the equation is numerically solved by using the finite element method. Due to similar principles, these conclusions can also be used to develop natural gas.

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Yao, J., Sun, H., Huang, Z., Zhang, L., Zeng, Q., Sui, Y., Fan, D.: The Key Mechanical Problems in the Development of Shale Gas. SCIENCE CHINA Physics, Mechanics & Astronomy 1527-1547 (2013)

Theoretical Analysis of Fracture Conductivity Created by The Channel Fracturing Technique Based on Homogenization

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ABSTRACT

The channel fracturing technique is a new technique in recent years. It can significantly increase fracture conductivity while reducing water and proppant consumption. It creates open channels inside the fractures, enabling hydrocarbons to flow through the stable channels rather than the proppant. However, the fracture conductivity calculation theory and related influence factors are not fully understood. In this study, an efficient model for calculating the effective permeability of channel-fracturing fractures is developed based on homogenization theory. Firstly, a simplified and physically-based deformation model of the channel-fracturing fracture subjected to constant confining stress is developed based on the elastic contact theory. And the coupled Darcy-Brinkman equations in fine scale are applied to evaluate the fracture's effective permeability. The proppant pillars are considered as the porous regions which are modeled by the Darcy equation, while the Brinkman equation is used for the flow in the open channels between pillars. Then, the upscaling of these equations from fine scale to coarse scale is implemented based on homogenization theory. The effective permeability of channel-fracturing fracture is obtained eventually to evaluate the fracture conductivity. Based on our model, sensitivity analysis including volume fraction of pillars, confining stress, pillars' distribution, etc. is conducted.

The adsorption and diffusion behaviour of CH4/CO2 in kerogen: A molecular simulation

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ABSTRACT

Kerogen is a chemically and physically heterogeneous organic matter usually occurring in shale strata in sedimentary rock. The nature of the constituents in kerogen derives from its source as well as later biochemical and geochemical processes. A van Krevelen plot based on elemental H/C data and O/C data shows the well established pattern for type I, type II, and type III kerogens [1]. In this work, The kerogen models unit are build by Ungerer [2] and make kerogen density is 1.0 g/cm3[3].
The adsorption isotherms of CH4/CO2 have been investigate by GCMC simulations at different temperatures, Adsorption behavior of both methane and carbon dioxide exhibit type-I Langmuir adsorption behavior[4], Langmuir equation can be used to fit for these isotherms. The temperature has a negative effect on gas adsorption, the adsorption amounts will decrease with increasing temperature at a given pressure. From the excess adsorption isotherms, there is a maximum adsorption for each temperature, suggesting there exists an optimum pressure for maximum methane storage at specific temperature. The self-diffusion coefficient of CH4/CO2 which is investigated by MD simulations combined with Einstein fluid equation increase with the temperature increase at same pressure. The self-diffusion coefficient decrease with the pressure increase at same temperature. The radial distribution function is used to study structural information of CH4/CO2 adsorbed in kerogen.

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Reconstruction of three-dimensional porous media model based on multi-point statistics method

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ABSTRACT

The traditional theory and experience based on the macro media model is fail to predict the fluid flow characteristics of shales, tight and other unconventional oil and gas resources reservoir accurately, the real structural characteristics of porous medium is one of key parameters for researching percolation mechanism. Hence it is necessary to reconstruct an effective description the rock matrix on the pore scale. In the paper, one novel method combining two-dimensional computed tomography (CT) scanning image with multi-point statistical (MPS) method, was presented to reconstruct a three-dimensional porous medium model. Multiple data template was used to scan two-dimensional computed tomography (CT) scanning image defined as training images in order to establish the search tree, the approach is not only conducive to express the feature parameters of macro and micro pore for anisotropy rock, but also helps to reduce storage space and improve simulation efficiency. In order to evaluate the accuracy of the reconstruction results quantitatively, the microstructure reconstructed by different methods including the novel method, Markov Chain Monte Carlo (MCMC) and computed tomography (CT) scanning method, was compared in the static parameters such as porosity, permeability, pore/throat size distribution, the results indicate that the microstructure reconstructed by multi-point statistical is superior to Markov Chain Monte Carlo (MCMC) methods, moreover it is in good agreement with computed tomography (CT) scanning method. Furthermore, the realistic network extracted from different microstructure were used to predict multiphase flow properties, the relative permeability estimated with MPS modeling are in good agreement with experiment.

Pore-scale simulation of viscoelastic fluid flooding using N-S equation

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ABSTRACT

Microscopic residual oil in reservoir after water flooding can be classified into three types: oil droplets, oil films, oil clusters. The main accepted mechanism of mobilizing residual oil after water flooding is that there must be a rather large viscous force to overcome the capillary forces. Viscous force cannot be increased by such a large magnitude in the field. Recently, viscoelastic fluid is widely applied in improving the recovery after water flooding in petroleum industry, and displacement efficiency is greatly improved. It's necessary to investigate how the viscoelastic fluid mobilizes the residual oil.

In this study,direct numerical simulation method is employed to simulate immiscible two-phase flows in porous media. The position of the interface between two immiscible fluids is determined by Phase Field method. Oil film and oil droplet in dead end dynamics are investigated under the condition of Newtonian and viscoelastic fluid displacement, respectively. Different wetting conditions of a reservoir rock are incorporated into the model. Interfacial tension between two fluids is calculated according to the CSF model. Viscoelastic effects are simulated using Oldroyd-B rheological model. The numerical solution used for the simulation was carried out by a finite element method.

Compared with the Newtonian fluid, viscoelastic fluid is easier to mobilize the residual oil which can greatly improve displacement efficiency. Both the normal stress and horizontal force acting on the residual oil films by viscoelastic fluids are much larger than Newtonian fluid. The viscoelastic fluids cause the residual oil droplet to deform significantly. Also, the wettability of rock wall has important impact on oil recovery. Water wetting reservoirs are more suitable for water flooding.

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Pressure-transient analysis of CO2 flooding in unconventional reservoir

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ABSTRACT

To analyze the pressure transient of CO2 flooding in unconventional reservoir, this paper proposed a transient flow model based on compositional model which can consider the wellbore storage effect, skin factor and multiple-contact process. Solve the model with finite volume method, and perform pressure transient analysis. The results show that the pressure derivative curve of the swept area radial flow raises first and then declines a little, the pressure derivative curve of the unswept area radial flow raises first and then becomes flat; the CO2 flood front can be recognized when the derivative curve begin to raise after it decline a little in swept area radial flow regime; the pressure and pressure derivative curves are sensitive to the injection time, injection rate, permeability, skin factor and wellbore storage effect which means that a numerical welltest interpretation method can be established based on the model used in this paper to estimate the permeability, miscibility, formation damage and monitor the CO2 flood progress.

Numerical simulation of ferrofluid flow in fractured porous media using the Galerkin finite element method

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ABSTRACT

Ferrofluids are suspensions of magnetic particles of diameter approximately 10 nm stabilized by surfactants in carrier liquids[1]. The large magnetic susceptibility of ferrofluids allows the mobilization of ferrofluid through permeable rock and soil by the application of strong external magnetic fields[2]. Because the ferrofluid flow in porous media can be controlled by magnetic field, there have a potential that using ferrofluid for flooding to raise the scope of the whole displacement to improve flooding recovery.

As we know, the progress of hydraulic fracturing technology has greatly promoted development of unconventional reservior. In this context, we have developed simulation capabilities for ferrofluid flow through fractured porous media in response to magnetic forces from the magnetic field to investigate the potential that using the ferrofluid for flooding in unconventional reservior. Fluid flow in the fractures is modelled explicitly by using discrete fracture model, which decreases the dimension of fractures and avoids calculating cross flow coefficient used in the dual continuum models [3].The magnetic force is introduced into the Darcy equation to coupling the magnetic field and seepage flow field, and the mathematical model is implemented using Galerkin finite element method. Validity and accuracy of the model and numerical algorithm are demonstrated through a 1-D horizontal tube example. At last, we compare numerical simulation results of the fluid pressures and the flow velocity in different fractured porous media model .

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Upscaling of gas transport in shale matrix based on Homogenization theory

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ABSTRACT

The shale matrix is composed of organic matrix with free gas and adsorbed, and inorganic matrix with only free gas. The gas transport mechanism in two different shale matrix is different. The conventional numerical model didn't consider the different gas transport mechanism in the shale matrix and the influence of the distribution of the organic matter. In this paper we established a upscaled shale matrix model with considering these mechanisms. In the microscale region, the Knudsen diffusion and viscous flow of free gas and surface diffusion of adsorbed gas is considered in the microscale model of organic matrix, while only Knudsen diffusion and viscous flow of free gas is considered in the microscale model of inorganic matrix. We calculated the production and pressure of shale matrix have different organic matrix distribution and same TOC content in the microscale region while have same parameters in the macroscale model, the result shows that the macro-scale equations solved directly without homogenization process have the same pressure and production while with upscaling process the solved pressure and production are different in these macro-scale models.

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Practical Solutions for flow behavior analysis in composite shale gas reservoir considering multiscale transport mechanisms

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ABSTRACT

Shale reservoirs are becoming more important in worldwide oil and gas production because of the use of multi-fractured horizontal wells. Shale gas reservoirs are composed of multiscale porous media (including porous kerogen, the inorganic matrix, natural fractures and hydraulic complex fracture network), it is necessary to consider the effects of multiscale transport mechanisms (slippage during viscous flow, Knudsen diffusion, surface diffusion) and distribution characteristics of complex fracture network. In this paper we incorporated a more detailed description of complex fracture networks to improve the pressure transient analysis of multi-fractured shale gas reservoir. In the proposed model, we represented the porosity and permeability of the fracture network in the Stimulated Reservoir Volume (SRV) using the fractal porosity–permeability relations. Specifically, we employed apparent permeability approach in which characteristics of flow in multiscale porous media are taken into consideration. We used an analytic multiple porosity media model to describe gas flow from kerogen to multi-fractured horizontal wells. Solutions for the MPM model were derived in the Laplace transform domain and then numerically inverted to the real time domain using the algorithm proposed by Stehfest. The solution was compared with the classic dual-porosity trilinear flow model for the special case, and the result revealed a perfect agreement between the solutions. Mass transfer between multiscale porous media were discussed in the paper, the results showed that the Vermeulen transient transfer model could described shale gas flow behavior more accurately than Warren-Root pseudo-steady state transfer model. The presented model was matched with actual data from multi-fractured horizontal wells in western China and the resulting curves can indicate the complexity of the fracture around the wellbore. At last, the effects of SRV parameters and fractal parameters on permeability distribution were performed. The model proposed in this study is more comprehensive, considering not only the complex fracture network characteristics of Stimulated Reservoir Volume but also the mechanisms of transport through media at multiple scales. Thus, this model is useful for performance analysis during shale gas reservoir development.

Experimental Investigation of Hot Water Injection to Enhance Oil Recovery of Tight Sandstone

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ABSTRACT

Flow of hot water will occur in all thermal enhanced oil recovery methods because the presence of water in all reservoirs. Oil viscosity decreases and oil mobility improvement play the most important part in enhance oil recovery in heavy oil reservoirs. Compared to heavy oil reservoir with high permeability reservoir, light oil flows in more complicate and heterogeneous pore structure in tight reservoir, which indicates that mechanism of hot water injection to enhance oil recovery is quite different.

Literature review shows the major mechanisms of thermal injection are viscosity reduction, thermal expansion, wettability alteration and oil/water interfacial tension reduction. To investigate the mechanism of hot water injection enhancing oil recovery, experiments were designed using field sandstone cores and light oil of tight reservoir, including oil properties, interaction between rock and fluid, petrophysical properties of the reservoirs. These experiments were conducted in reservoir pressure but in various temperature ranges up to 150?. Also, threshold pressure gradient, relative permeability curves and oil recovery were obtained from core scale displacement experiments.

Results show that: with increasing temperature, oil-water viscosity ratio falls slightly which has little effect on oil recovery and this is definitely different with thermal injection in heavy oil, the volume factor of formation oil increases significantly which can highly supply the formation energy and raise the formation pressure, oil/water interfacial tension decreases slightly which has a positive effect on increasing production though the reduction is not obvious, core samples analysis show that the pore characteristics turns better. Meanwhile, the irreducible water saturation and the residual oil saturation are both reduced, the common percolation area of two phases is widen and the general shape of the curve turns better; the threshold pressure gradient decreases related power function with the temperature which all indicate that liquid flows easier in porous media and the effect of water displacement becomes better. Actually, oil recovery is raised due to all these factors.

Quantitative experiments data show that all factors discussed influence the flow of two phases in porous media. It is obvious that there is a distinct difference of the dominant mechanisms of hot water injection to enhance oil recovery between tight and heavy oil reservoirs. The study may provide a reference for hot water injection in tight reservoir.

Automatic History Matching Considering Viscous Fingering in Naturally Tight Fractured Reservoirs

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ABSTRACT

For naturally Tight fractured reservoirs, there are huge quantities of natural fractures and viscous fingering would be more unstable because of those fractures, in turn, the viscous fingering flow in matrix and fractures would make great impact on the efficiency of enhanced oil recovery, heavy oil production process and carbon sequestration application [1]. We present a new approach for high-fidelity history matching considering viscous fingering in naturally tight fractured reservoirs. The history matching method is based on an automatic algorithm by adjusting fracture location, orientation and length in a dynamic state. In the process of simulation, one of the key features of the proposed method is considering the impact of changes in viscosity and relative permeability on multiphase flow, the other is dealing with the discrete fractures as embedded objects into the matrix [2]. The present formulation solves pressure and transport equation by finite element method which is developed for coupling the embedded fractures and matrix. The history matching results demonstrate the accuracy and robustness of the method and some interesting phenomena associated with high conductivity of fractures are simulated, such as the increasing of the growth rate of viscous fingers and the alteration of flow patterns near fractures.

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Pore-network modelling of two-phase flow and transport in porous media

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ABSTRACT

Among different pore-scale modelling approaches, pore-network modelling is still the oldest one and the most common one. Thanks to its less expensive computational costs, much larger physical scales can be simulated using this approach compared to the other ones such as Smooth Particle Hydrodynamics, Level Set, Lattice Boltzmann, or Direct two-phase Navier-Stokes simulations. This talk provides an overview of wide applications of pore-network modelling for different applications such as two-phase flow, solute transport, and two-phase transport in porous media. Micro-scale and column scale experimental results are provided to show the capability of such models in simulating complex problems. In this presentation a multi-process pore-network model is provides where solute transport under two-phase conditions is presented. The results are significantly important for vadose zone contaminant transport as well as enhanced oil recovery applications.

Modelling the dynamics of capillary effects on the pore-scale for low capillary numbers

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ABSTRACT

Multiphase flow in porous media is mainly influenced by capillary effects [1]. Therefore, the Navier-Stokes equations must be extended to account for interface and contact-line phenomena. For the description of surface forces, the Continuum Surface Force model (CSF) is used together with the Contact Line Force model (CLF) [2], which was recently introduced to describe wall-fluid-fluid interactions. This approach uses the non-compensated Young force to model contact line dynamics and therefore uses a similar extension to the Navier-Stokes equations like the CSF model.
The CSF/CLF model was used with the computational method smoothed-particle hydrodynamics to simulate a drainage process in a porous structure and the results have been compared with a corresponding micromodel experiment. While the flow path is in good agreement, the dynamics of simulation and experiment differ clearly [3]. It was found that this deviation increases when the drainage takes place at low capillary numbers. In former wetting experiments an additional resistance on the contact line called “stick-slip” [4] was found in cases when wetting takes place on rough surfaces at low capillary numbers. This behaviour can’t be captured in the current CSF/CLF model.
In this work the combined CSF/CLF model is extended in order to describe wetting processes at low capillary numbers. Simulations of different wetting processes are compared with experimental results.

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Phase pressure distribution and its effects on multiphase flows in porous media

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ABSTRACT

We simulated two-phase immiscible displacements in a porous medium using a multiphase lattice Boltzmann model. The displacement was driven by a constant pressure differential applied to the inlet and outlet of porous medium. As the pressures of phases can be directly obtained from the simulations, we were able to track the evolution of the pressure distributions inside the porous media during imbibition and drainage. When the capillary number is low, significant differences between the pressures of non-wetting and wetting phases are observed. At the front of displacement during drainage, a lower pressure difference between the two phases is observed, because the non-wetting phase first displaces the wetting phase in larger pores where the capillary pressure is low. On the contrary, there is a high pressure difference at the displacement front during imbibition because the wetting phase occupies smaller pores first, where the capillary pressure is the most significant. After breakthrough, the pressure gradients of the two phases gradually became identical in both drainage and imbibition processes. Relative permeability is then modeled using the actual pressure gradient of each phase at different times. This work provides an insight into the role of pressure in driving multiphase flows through porous media.

Simulation of two-phase flow micro-model experiments using Volume of Fluid method

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ABSTRACT

Micro-scale two-phase flow experiments[1]are simulated using Volume of Fluid method[2]. Distribution of fluid with time from simulation is compared with observed flow pattern in experiments. Disagreement between simulation and experiments are found. Explanations are given based on simulation of extra single phase and two-phase flow experiments[3], [4].

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Impact of mineral grain surface roughness on CO2 ganglion dynamics

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ABSTRACT

Capillary trapping and migration of supercritical CO2 (scCO2) ganglia associated with geologic carbon storage is strongly dependent on wettability, which is characterized by the contact angle of scCO2 on mineral grain surfaces, and in turn depends on mineral surface composition and roughness. Natural and reaction-induced surface roughness on mineral grains also impacts the effective permeability of pore fluids in low porosity porous materials. Our ganglion dynamics model has shown that capillary trapping and buoyant movement of scCO2 ganglia highly depends on the wettability (contact angle) of scCO2 on mineral grain surfaces (Wang et al., 2012). Surface roughness plays a key role in engineering of super-hydrophobic solid surfaces for industrial and consumer applications. We extend this concept to actual mineral surfaces to understand the effect of mineral surface roughness on the contact angle of scCO2 and the effective permeability to flow. Using the Cassie-Baxter theory (Cassie and Baxter, 1944), we have calculated the apparent contact angle of rough mineral surfaces from the contact angle measured on a smooth planar surface. Moreover, injection of scCO2 into a brine-saturated reservoir alternately involves drainage (injection) and imbibition (buoyantly-driven CO2 migration), wherein brine or scCO2 may alternatively become trapped on the heterogeneous surface roughness of mineral grains. This strongly impacts reservoir permeability in low porosity media. Using computational two-phase fluid dynamics we assessed the impact of surface roughness on the effective permeability of these pore-scale flows, which has a strong influence depending on the flow configuration (imbibition or drainage), fluid wettability, viscosity ratio and roughness characteristics. The effect of surface roughness has been incorporated into our ganglion dynamics model. Our preliminary modeling result shows that mineral surface roughness can have a significant effect on scCO2 ganglion trapping and mobilization.

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Pore-scale Analysis of Gas Flow in Mixed-wet Shale Matrix Systems

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ABSTRACT

Shale formations have been key to the unconventional energy revolution and, more recently, have been considered as potential CO2 storage sites. The complex properties of shales that distinguish them from typical geo-materials are nano-scale pore sizes, low permeability, low connectivity and mixed components (inorganic matrix with organic regions). Nano-scale flow paths lead to flow regimes such as slip flow and Knudsen diffusion, which differ from viscous flow and can play a dominant role during shale gas production. Sorption in organic regions of the rock is also an important process. Furthermore, the water in shale formations leads to a two-phase flow system (Huang et al., 2015). Inclusion of all of these factors in a pore-scale model may provide a promising way to improve understanding and to optimize shale gas extraction.

Pore-network modeling is now a practical way to explain the macro-scale flow behavior of many porous media from a microscopic (pore-scale) point of view (Joekar-Niasar et al., 2010). In this work, a three-dimensional pore-network model is developed to simulate gas flow in a mixed-wet shale matrix, in which the typical bimodal pore size distribution in shale is included (Zhang et al., 2015). In addition, a new dilution algorithm is proposed for the pore-connectivity of shale matrix, which can flexibly account for the low connectivity of the pore-structure. The gas flow is simulated in the extracted pore network backbone, which is reasonable in gas extraction, as many isolated pores exist in shale matrix. For the models presented herein, pore bodies are sphere-shaped, and pore throats are cylindrical. We consider different fluid displacement scenarios, including water invasion and then subsequent gas production. Local relations between capillary pressure and saturation (Pc-Sw) in pore bodies are established to reflect different invasion mechanisms and models within single pore bodies. We simulate dynamics of invasion, and use a modified algorithm where multiple pore elements can be filled during one time step. This is much more efficient for pore network simulation of fluid flow in porous media than earlier models that require only one pore filling per time step.

We report on sensitivity analyses focused on the impact of average coordination number, pore-throat size, and desorption in kerogen. We also consider differences in simulation results based on local capillary pressure rules within individual pore bodies.

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X-ray microtomography imaging of immiscible fluids after imbibition: a multi-resolution dataset

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ABSTRACT

The security of CO2 sequestration in underground formations relies on the efficiency and long-term reliability of the trapping mechanisms occurring in the reservoir where CO2 is injected. One major process for storage security beyond the primary stratigraphic seal is residual (capillary) trapping. It is often assumed that the resulting disconnected ganglia, trapped phase, are permanently immobilized in the pore network. However multiple mechanisms such as further dissolution in brine, wettability changes, or Ostwald ripening, may lead to fluid phase redistribution and thus possible remobilization of residually trapped CO2.
The aim of this work is to quantify fluid phase distribution and connectivity and capillary pressure distribution in the trapped phase in order to assess potential changes in fluid phase organization with time. A multi-scale synchrotron-based X-ray microtomography dataset was acquired in sintered glass beads and sandstone samples with voxel sizes varying from 0.64 to 4.44 µm. In each case, the non-wetting and wetting phase were indentified, as well as their interface, and capillary pressure was measured using calculation of interfacial curvature. The results show that most residual ganglia display similar capillary pressure, apart from small bubbles localized in one pore body, which present higher values but account however for less than 0.2% of the total residual phase. The comparison between different resolutions for a same experiment highlights the sensitivity of the chosen voxel size on fluid phase identification and capillary pressure calculation. This complete dataset represent a great opportunity for direct numerical modeling of multiphase flow in different pore network structures.

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Velocity fluctuations in flow through porous media

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ABSTRACT

Modeling and quantification of velocity fluctuations is essential to fully understand the flow behavior at the pore-scale, but it is neglected in continuum approaches using Darcy's law. In this study, we investigate the spatial flow fluctuations of a slow flow through porous media on the pore scale using a combined numerical simulation and experimental approach. We perform direct numerical simulations of flow through arbitrary porous geometries in conjunction with particle image velocimetry to obtain flow characteristics at the pore-scale. Velocity correlations and probability density functions of velocity components are evaluated for both single phase and multiphase flow through porous media. The immerse boundary method and volume of fluid approach are used to capture pore structure and oil water interface, respectively. 2D time-resolved flow measurement at high spatial resolution is obtained by micro-PIV within a monolayer glass bead flow channel. Special efforts are made towards simultaneous two-phase flow measurement to capture the interfacial interactions. Fluorescent seeding particles with different emission peaks are used for aqueous and oil phases. The flow channel is fabricated using borosilicate glass cell and hydrophilic transparent glass beads. The geometry of the flow channel is reconstructed from a high resolution micro-CT scanner and is used for numerical simulation. By direct comparison of the result from PIV measurement and direct numerical simulations in exactly the same geometry, we are able to study the influence of porous media properties such as porosity and pore size distribution on fluid transport at micro-scale, crucial to many areas such as contaminate migration and enhanced oil recovery.

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An Integrated Workflow from FIB-SEM Digital Imaging to DPD Mesoscale Multiphase Flow Simulation in Organic-Rich Nanoporous Shales

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ABSTRACT

Numerical modeling & simulation of nano-pore-scale fluid flows is an important approach for enhancing the fundamental understanding of flow and transport phenomena in fine-grained organic-rich nanoporous shales. The flow simulations for problems of practical interest (e.g., in a micro-scale shale rock sample) is, however, too computationally expensive for a molecular dynamics (MD) model, and far from mature in theory for a continuum computational fluid dynamics (CFD) model. In fact, it is a longstanding challenge due to the multi-length-scale nature of the shale pores that can range between the nano-scale (1E-9 m) and micro-scale (1E-6 m). Recently, the dissipative particle dynamics (DPD) models, which were originally developed for microscopic hydrodynamics, have been extended for mesoscale fluid flows in porous media. A remarkable feature of the DPD models is that they are able to reproduce some of the key characteristics of fluid flows at both the molecular and continuum scales, which make those models more flexible and affordable for a multi-scale system. Among the various DPD models, the Warren's many-body DPD (termed MDPD) method has been found particularly suitable for multi-fluid systems, and relatively simple to parameterize for specific types of fluids. However, compared with the advancement of MDPD in its theoretical aspects, the application of MDPD for flow simulation in pore-scale shales is relatively less explored, mainly due to the lack of the structural and material information that needs to be obtained from the shale rock samples. In the present work, a seamless workflow combining a focused ion beam scanning electron microscopes (FIB-SEM) digital imaging technique and an MDPD flow modeling & simulation approach will be introduced for the numerical study of mesoscale multi-phase/multi-fluid flows in heterogeneous nanoporous shales. In the full paper, we will first overview the MDPD method, including the formulation, advantages & disadvantages, and limitation of applicability in micro- / sub-micro-scale geological porous media. To provide sufficient geometric information for the MDPD simulations, we will then introduce the FIB-SEM digital imaging procedures of organic-rich shale rock samples (see Graphic 2), post-processing of the imaging data, and reconstruction of the nanoporous environment using the general DPD particles. Finally, several numerical study cases will be reported. In those numerical problems, the highly nonlinear behavior of fluid flows in nano pores will first be demonstrated by the simulated dependence of solid–liquid dynamic contact angles on the characteristic pore size, which has been found to largely deviate from the classic continuum laws (see Graphic 1). The examples of multi-fluid flows in real organic-rich shale pores, where the geometries have been obtained from FIB-SEM digital imaging (see Graphic 3), will then be presented to demonstrate the capability of the developed workflow. Note that neither the particle based simulation, nor FIB-SEM is completely new to the area of pore-scale modeling and experiment on multiphase flow in porous media. Nevertheless, the present approach that integrates the FIB-SEM imaging into the DPD modeling & simulation for fluid flows in organic-rich shales is relatively new toward developing a robust, accurate, and ultimately competitive pore-scale model to bridge the gap between the molecular- and grain-scale.

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Wall effects in the sedimentation of micro- and nano-particulate swarms within fractures: combined insights from experiments and computer simulations

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ABSTRACT

Motivated by applications in subsurface contamination by micro- and nano-particulates through fracture pathways, this paper combines laboratory experiments and numerical simulations to examine the sedimentation of particle swarms at low Reynolds number and confined by planar and rough walls. Coherent evolution and breakup of particle swarms is similar to the behavior observed for miscible drops of liquid (i.e., having negligible interfacial tension). This analogy is grounded in theory, and serves as a baseline against which granular effects can be contrasted. In particular, however fine the particulate "discretization", significant statistical variations in time and distance to destabilization can be observed for macroscopically equivalent initial drop shapes [1]. Furthermore, the collective sedimentation is significantly enhanced within an optimal range of apertures. The experiments advance beyond previous investigations of single-wall and double-wall configurations [1,2] in treating realistic roughness of fracture apertures. Numerical simulations track swarms of point-particles that mutually interact through their (regularized) Stokeslet fields. A P^3M technique accelerates the summations for swarms exceeding 10^5 particles [3]. Wall effects are incorporated using a least-squares variant of the method of fundamental solutions, with grid mapping of the surface force and source elements within the fast-summation scheme [4,5]. To facilitate comparisons of simulations with experiments, the laboratory images are mathematically processed to obtain accurate three-dimensional initial swarm configurations to launch the simulations.

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Dissipative Particle Dynamics Simulations of Multiphase Flow in Nanoporous Media

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ABSTRACT

An adequate understanding of multiphase flow in nanoscale pores is important for enhancing the fundamental understanding of flow and transport phenomena in the fine-grained nanoporous shales. However, in terms of computer modeling, it is still either too expensive to use a molecular dynamics (MD) based model, or far from valid to use a continuum mechanics based computational fluid dynamics (CFD) one for flow simulations in shale pores, due to the multi-lenghscale nature
of shale pores that can range between the pore scale (10?9 m) and grain scale (10?6 m). Instead, a mesoscale flow model such as the dissipative particle dynamics (DPD) stands as a potential candidate, as it is able to reproduce some basic aspects of both the molecular- and continuum-scale mechanics. In the present work, several typical scenarios of fluid statics and dynamics in slit
pores of a few nanometers wide are studied by the many-body DPD simulations. Analysis of the dependence of solid–liquid static contact angle on the pore width shows a highly nonlinear behavior of the liquid demonstrates in terms of the wettability, which largely deviates from the prediction by the Young's law. It is observed that in the forced displacement of liquid–liquid (l–l) interface, different injection fluid mass fluxes can result in quite unique l-l interface shapes and
even induce "fingering" instability in a wider pore, whereas it does not cause discernible difference in narrower pores. Notably, a halved pore width can result in a significantly slower l–l interface displacement and excessively stronger fluid pressure, though subject to the same inflow mass flux. Those nonlinear static and dynamic flow behaviors observed provide some guidance for both the numerical simulations and lab experiments of fluid injection into nanoporous shale rock samples.

Modelling of polymer membrane formation using Smoothed Particle Hydrodynamics

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ABSTRACT

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.
Since the dynamics are driven by mesoscale effects fluctuating hydrodynamics have to be considered. One mesoscale method including fluctuations is the Smoothed Dissipative Particle Dynamics (SDPD). We present a SDPD model including surface tension and investigate gradients in surface tension that could be responsible for defects in polymer membranes and macrovoids. Numerical results are compared with experiments.

Pore-Scale Network Modeling of Water Transport in the Micro Porous Layer and Gas Diffusion Layer of a Polymer Electrolyte Fuel Cell

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ABSTRACT

For optimal water management of a polymer electrolyte fuel cell (PEFC), it is crucial to understand the transport mechanisms of water throughout the cell constituents. Over the past few years, pore-scale modeling of diffusion layers and gas channels has attracted much attention.
In this presentation, a recently developed dynamic pore-network model is presented [1]. The model explicitly solves for both water pressure and capillary pressure. A semi-implicit scheme is used in updating water saturation in each pore body, which considerably increases the numerical stability at low capillary number values. Furthermore, a multiple-time-step algorithm is introduced to reduce the computational effort.
A number of case studies of water transport in the micro porous layer (MPL) and gas diffusion layer (GDL) are conducted. We illustrate the role of MPL in reducing water flooding in the GDL. Also, the dynamic water transport through the MPL-GDL interface is explored in detail. This information is essential to the reduced continua model (RCM), which was developed for multiphase flow through thin porous layers [2, 3].

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Injection of CO2 into Brine-Saturated Porous Media - Micromodel Experiment and LBM Simulation

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ABSTRACT

The sequestration of carbon dioxide into geological formations has been an alternative to mitigate the global climate change. The capillary trapping among other storage mechanisms such as dissolution trapping and mineral trapping occurs when injected CO2 displaces brine in pore space so that CO2 remains trapped in pore space. The efficiency of CO2 displacement is dependent on both controllable (i.e., fluid viscosity and surface tension, injection rate) and uncontrollable factors (i.e., pore network, wettability, pore surface roughness). Among these factors, we focus on the influence of injection conditions by controlling the injection rate and the phase of fluids invading into a 2D microfluidic chip in order to quantitatively assess the displacement ratio. The injection rate varies three orders of magnitude (i.e., 1, 10 and 100 muL/min) for each of the four invading fluids including gaseous, liquid, supercritical CO2 and CO2 droplet-in-water Pickering emulsion. High-resolution digital images are consecutively captured until no volume change of brine is observed and subjected to the series of image analyses. Five runs are performed under the same experimental conditions to obtain statistically reliable values. The injection rate and the viscosities of invading fluid and brine uniquely define the capillary number (C) and the viscosity ratio (M), and the resultant replacement ratios are compared with previously reported values in logC-logM space. Furthermore, the implementation of Lattice Boltzmann Method (LBM) allows numerically assessing the displacement ratio of CO2 within the same domain of 2D microfluidic chip. Both experimental and numerical studies commonly exhibit the phase-dependent spatial configuration of injected CO2 and different displacement ratio. Results highlight that the saturation of injected CO2 can be controlled by manipulating the injection rate or the invading fluid phase to optimize the storage capacity with the in-situ applicability.

Impact of Pore Scale Heterogeneity on Interphase Mass Transfer in Porous Media

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ABSTRACT

Interphase mass transfer in porous media is observed in numerous industrial and environmental applications. It is often determined from laboratory experiments conducted at the meso-scale. The interpretation of these experiments is generally expressed in terms of Sherwood number correlations that relate the interphase mass transfer to average fluid and porous media properties. Although these relations assume uniform flow and porous media properties, in reality natural porous media are almost always heterogeneous. In this study a pore-network model is developed to examine the influence of pore-scale spatial variability on interphase mass transfer. A Monte Carlo approach was used to generate multiple realizations of the porous media with spatially variable grain size distributions. For each realization the flow field is simulated for different fluid pore-scale configurations and used to compute the probability density functions of the mass transfer coefficient- both explicit and lumped- and the corresponding Sherwood number expressions. It is shown that pore-scale heterogeneity of the porous media and the corresponding pore-scale fluid distributions strongly influence interphase mass transfer. The implication of these finding on real life applications are discussed.

Influence of dynamic factors on non-wetting fluid snap-off in pores

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ABSTRACT

Snap-off is an important dynamic multiphase flow phenomenon which occurs in porous media. It plays a dominant role in the residual trapping and mobilization/immobilization of non-wetting fluids such as hydrocarbons or CO2. Current studies, applications, and threshold criteria of snap-off are mostly based on static or equilibrium conditions. Thus, the dynamics of snap-off which is relevant for many real world applications has rarely been systematically studied. While a static criterion indicates the snap-off potential for non-wetting fluids, the competition between the time required for snap-off and the local pore throat capillary number determines whether snap-off actually occurs. Using a theoretical model to couple the wetting film thickness to the local capillary number at the pore throat, we analyzed the dynamics of the wetting/non-wetting interface instability in sinusoidally constricted capillary tubes. The influence of dynamic factors as encapsulated by the effect of local capillary number on non-wetting fluid snap-off time were investigated for varying pore throat to pore body aspect ratio and pore body distances. The analysis showed that snap-off can be inhibited by a sufficiently large local capillary number even in cases where the static snap-off criterion has been met.

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Biosurfactant-facilitated hydrocarbon displacement in porous media: A micromodel study

Presenter: Daniel Hayward
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ABSTRACT

During the process of immiscible displacement of a receding fluid (e.g. oil) by an invading fluid (e.g. water) in porous media, one or more pores may be bypassed by the invading fluid as it advances through the medium. This process creates disconnected fluid clusters which are left behind, trapped in the porous structure [1-2]. Developing novel approaches for removal of those disconnected and trapped fluids from porous media is of great importance in many processes such as enhanced oil recovery [3] or the design of efficient remediation schemes for sites contaminated with petroleum-based products. This motivated many researchers to investigate the efficiency of various injecting fluids such as foam, water, gas, or surfactants on mobilising and removal the trapped fluids. Surfactants for soil remediation must have low toxicity to prevent further aggravation of the problem. Biosurfactants are surface-active substances that are formed by biological cells. These compounds have the ability to reduce surface tension and interfacial forces where liquids, solids and gases interact. This gives them great advantages as surfactants can mix or diffuse easily in emulsions, whether this is water or in another fluid. Biosurfactants have multiple advantages over more commonly used chemical surfactants. They are biodegradable and non-toxic, hence ecologically safe, and are found to be effective at extreme temperatures and pH levels. Due to the reduced toxicity levels that biosurfactants show we have been motivated us to manufacture and use them in our investigations. The objective of this work was to evaluate the performance of in-house synthesized biosurfactants (sophorolipids) in oil recovery from 2D porous media. To do so, we have conducted micro-fluidic experiments using micromodels fabricated based on X-Ray computed tomography images of a sand-pack with varying grain sizes leading to a more realistic pore network representation. The micromodels were fabricated in a silicon wafer using standard photolithography and inductively coupled plasma–deep reactive ion etching methods. The micromodel was first saturated with a 10 cps silicon oil followed by biosurfactant flooding (1% concentration) at a defined flow rate. The dynamics and patterns of the interface displacement as well as the size distribution of the trapped oil ganglia were visualized using an optical microscope equipped with a high resolution CCD camera. Image J software was used to analyse the images to obtain the recovery factor and the size distribution of the trapped oil as a function of the permeability of the porous media. The experiments were repeated for water and Triton X100 surfactant to compare the effectiveness of biosurfactant performance compared to the other two fluids. Using the obtained pore-scale information, the effect of the porous media properties on the trapping of oil during water, biosurfactant, and surfactant flooding was demonstrated. The potential environmental benefits of biosurfactant over chemical surfactant, generally used in the surfactant remediation processes, are illustrated.

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Comparison of lattice Boltzmann method and pore-network modeling of CO2 and brine flow in Mt Simon Sandstone

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ABSTRACT

Understanding CO2 and brine flow at the pore-scale and predicting flow and transport properties is vital in geological storage of CO2. The complex geometry and heterogeneity of geological formations requires using relatively large samples to ensure having representative elementary volume at the pore-scale. Pore-network modeling (PNM) works based on ideal equivalent geometry with simplified equations of flow in pore throats and capillary pressure equation in pore bodies. It can be used on fairly large samples with efficient computation cost. On the other hand, the Lattice Boltzmann Method (LBM) recovers the Navier-Stokes equations on real geometries, but is computationally expensive and cannot be used on large samples. Therefore both methods have advantages and disadvantages, and it is worthwhile to compare their application on real samples.

In this study, micro computed tomography images of Mt Simon Sandstone provided by the National Energy Technology Laboratory will be processed to identify pore spaces and solid grains. The geometry will be used directly by LBM to determine flow characteristic curves, such as relative permeability and capillary pressure. For pore-network modeling, an equivalent three-dimensional network will be extracted including spatial properties of pore bodies and pore throats. Then a quasi-static pore-network model will be used to simulate drainage and imbibition processes and determine characteristics curves. This analysis will be done on different subsamples from Mt Simon Sandstone to compare topological properties of subsamples, and have better understanding how small scale heterogeneities affect the LBM and PNM results.

This work is primarily supported as part of the Center for Geologic Storage of CO2, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science and partially supported by the International Institute for Carbon-Neutral Energy Research (WPI-I2CNER) based at Kyushu University, Japan.

The impact of dual porosity on steady state pore-scale fluid distributions, wetting phase connectivity and relative permeability

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ABSTRACT

The last 5 years have seen a rapid advance in the ability of petroleum scientists to examine reservoir processes directly at the pore scale, principally through coupling Special Core Analysis (SCAL) techniques with non-invasive x-ray micro-CT imaging1. These techniques have been used to investigate processes such as trapped gas saturation2, wettability changes and even dynamic multiphase displacements3. Such experimental developments have, however, not typically focussed on relating flow behaviour to the pore structure of the host rock. In this study we present the first comparison of steady state core-flood experiments, conducted at reservoir conditions and imaged at the pore scale with resolutions of around 4.5 μm. Experiments were conducted in two qualitatively different pore structures; a single porosity sandstone and a dual porosity carbonate.

During steady state fluid flow the single porosity sandstone showed a well-connected wetting phase flow path. The carbonate, however, showed the wetting phase to be poorly connected through the macroporosity. Wetting phase flow (and so relative permeability) can only be explained by including connectivity through the microporous network. A multi-scale computational model was constructed which was able to reproduce the measured relative permeability of the carbonate better than when the model was constructed using macroporosity alone. The multi-scale model was created by populating microporosity from the micro-CT images with permeabilities modelled from high resolution nano-tomography images (with voxel sizes of around 50nm), proscriptively sampled from microporous regions.

This work has important implications for the characterization and modelling of flow in such systems. It is often assumed that microporosity, while important for volumetric petrophysical measurements (such as fluid saturation), has only a minor contribution to displacement and flow, as the permeability of the microporous network is often much lower than the permeability of the macroporous network. For this reason it is frequently ignored. This assumption makes pore-scale modelling of petrophysical properties much more computationally efficient, however may not capture physics critical for multiphase flow in dual porosity rocks. The ability to conduct full steady state core-flooding experiments, imaged at the pore scale, shows the difficulty of such assumptions, and the value of a full multi-scale description of pore structure.

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Pore-scale Simulations of Capillary Trapping of Supercritical CO2 after Multiple Drainage and Imbibition Cycles

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ABSTRACT

Carbon capture and storage (CCS) of carbon dioxide emissions generated by production or combustion of fossil fuels is a technologically viable means to reduce the build-up of CO2 in the atmosphere and oceans. On a fundamental level, capillary trapping of scCO2 is a pore-scale process that shares mechanisms that are relevant, for example in oil recovery and remediation of NAPL-contaminated aquifers. Capillary trapping of scCO2 differs rather significantly from trapping of oil recovery and NAPL remediation in that the goal is to maximize the amount of NWP storage, whereas the objective of the other applications is to minimize the amount of residual NWP. This difference makes research into capillary trapping of scCO2 unique, but also complex because scCO2 phase properties (e.g. viscosity, density, and interfacial tension) exhibit large shifts with pressure and temperature which can strongly alter the trapping potential and efficiency. In this presentation we compare direct pore-scale observations of the Brine-CO2 drainage and imbibition process with lattice Boltzmann model simulations. The observations were conducted with the synchrotron-based x-ray microtomography facility at the Advanced Photon Source (APS) at Argonne National Laboratory using a novel x-ray compatible, high-pressure, elevated temperature setup. The “large” volumes (~1200 mm3; 6.3 mm diameter and 40 mm in length) were segmented into solid phase (Bentheimer Sandstone), Brine (KI, 1140 kg/m3) and scCO2. We will present LB simulations of small (64^3 voxel) and large sections of the scanned cores with a simple Shan-Chen-type model and a more advanced Equation of State-type model and compare model results to pressure and CO2 saturation levels that were observed for the CO2 invasion and Brine re-imbibition process. We will present results for the smaller sections under multiple drainage and imbibition cycles to investigate whether this will lead to enhanced trapping of scCO2 as found in earlier research.

Effects of Shear-thinning Fluids on Residual Oil Formation in Microfluidic Pore Networks

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ABSTRACT

Two-phase immiscible displacement in porous media is controlled by capillary and viscous forces when gravitational effects are negligible. The relative importance of these forces is quantified through the dimensionless capillary number Ca and the viscosity ratio M between fluid phases. When the displacing fluid is Newtonian, the effects of Ca and M on the displacement patterns can be evaluated independently [1,2]. However, when the injecting fluids exhibit shear-thinning viscosity behaviour the values of M and Ca are interdependent. Under these conditions, the effects on phase entrapment and the general displacement dynamics cannot be dissociated. In the particular case of shear-thinning aqueous polymer solutions, the degree of interdependence between M and Ca is determined by the polymer concentration. In this work, two-phase immiscible displacement experiments were performed in micromodels, using shear-thinning aqueous polymer solutions as displacing fluids, to investigate the effect of polymer concentration on the relationship between Ca and M, the recovery efficiency, and the size distribution of the trapped non-wetting fluid. Our results show that the differences in terms of the magnitude and distribution of the trapped phase are strongly influenced by the polymer concentration which influences the values of Ca and M.

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Pore scale simulation of soil hydraulic and thermal properties using phase field method

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ABSTRACT

Understanding the partitioning of water and energy fluxes in soil is important to many hydrological, agricultural and industrial applications. Although it is well known that heat and soil moisture fluxes through the subsurface create variations in both hydraulic and thermal conductivity, especially in unsaturated soil near the soil surface, our understanding of how to properly implement this behavior in numerical modeling efforts at the representative elementary volume (REV) scale is often limited due to a lack of understanding of the pore scale processes. For instance, effective thermal conductivity oftentimes included in numerical models through the use of empirical relationships and simplified mathematical formulations developed based on experimental data obtained at either small laboratory or field scales. In most of these models, local thermodynamic equilibrium between the air and water phases for a REV is assumed. However, this assumption may not always be valid at the pore scale, thus questioning the validity of current empirical relationships. The purpose of this work is to improve upon the relationships developed at the REV scale through simulating the thermal conductivity-saturation relationship and water retention curve of coarse-grained sands at the pore. A numerical model based on the coupled Cahn–Hilliard and heat transfer equation was developed to solve for liquid flow and heat transfer through variably saturated porous media. In this model, the evolution of phases and the interfaces between phases are related to a functional form of the total free energy of the system. The energy-based variational formulation of the phase field method allows for the incorporation of complex geometries and sharp solid interfaces. A unique solution for the system was obtained by solving the Navier-Stokes equation through free energy minimization. The simulated water retention curve was in a good agreement with experimental results especially in lower saturations. Simulations of the thermal conductivity-degree of saturation relationship showed that water-grains pathways are highly conductive of heat and are most likely responsible for the abrupt decrease in thermal conductivity when saturation drops below a certain threshold. Overall, results of these simulations can be used to assess the validity, limitations and accuracy of current models for estimation of thermal conductivity of soil at different saturations and temperatures.

Pore-Scale Multiphase SPH Study on Wetting Phase Entrapment during Primary Drainage in Particulate Media

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ABSTRACT

Assessing the stability and evolution of saturation fronts, or, from a microscopic point of view, interfaces between immiscible bulk fluid phases, is key with respect to design and control of subsurface processes such as sequestration of carbon dioxide in geological media or enhanced oil recovery. Depending on the governing capillary number Ca and viscosity ratio M, flow of immiscible fluids in porous media may exhibit macroscopic patterns as diverse as viscous fingering, stable displacement or capillary fingering. Yet, contemporary macroscopic models for two-phase flow assume the same set of governing balance equations (extended Darcy law, saturation mass balance) and conceptually equivalent constitutive equations (relative permeability function, capillary pressure function) applicable to all displacement patterns. The latter inherently assumes the associated pore-scale physics to be equivalent. We present pore-scale resolved direct numerical simulations (Sivanesapillai,2015) of primary drainage in porous media of particulate microstructure for various points of the (Ca,M) phase diagram. In an attempt to meet the question, whether or not pore-scale flow topologies associated with different displacement patterns are equivalent, we characterize the entrapment of wetting phase.
Our results show that, for viscous fingering, i.e. when Ca>10^2 and when the viscosity of the invading fluid is considerably lower than that of the defending fluid, fluid displacement at the pore-scale is reminiscent of Bretherton's problem, i.e. flow of gas bubbles in saturated capillary tubes. The corresponding flow topology is such that the less viscous fluid drains through the core of a pore-throat causing the formation of wetting films absent of contact lines on solid surfaces; ultimately rendering non-equilibrium momentum exchange between both fluid phases non-negligible. The latter casts doubt on the classical use of relative permeability functions, which, by definition, are related to momentum exchange between solid and fluid phases only. For stable displacement, i.e. when Ca>10^2 and when the viscosity of the defending fluid is considerably lower than that of the invading fluid, saturation profiles evolve by what might be referred to as travelling shock wave - a well known solution to the Buckley-Leverett (BL) equation. However, rather than being sharp as predicted by the BL equation, pore-scale simulations reveal the saturation front to be diffuse. Pore-scale flow topology within the diffuse zone, or, also referred to as capillary dispersion zone, is observed to exhibit complex events such as frequent fragmentation and coalescence of hydraulically isolated wetting clusters. The latter casts doubt on the purely hyperbolic BL equation. For capillary fingering, i.e. when Ca<10^4, fluid displacement is reminiscent of invasion percolation with frequent pore-scale events singular in time, such as Haines jumps and associated velocity bursts (Berg,2013). The evolution of interfaces during capillary fingering is governed by a scalar energy balance comprised of pressure-volume work and interfacial tension-interfacial area work. Trapping of wetting phase is primarily observed in high-curvature domains that are inaccessible to percolation. The latter casts doubt on coarse-grained models that do not explicitly take into account the evolution of interfacial areas (Hassanizadeh,1990).

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Wettability shifts caused by CO2-brine-rock interactions

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ABSTRACT

In geologic carbon sequestration applications, CO2 wetting on mineral surfaces will impact capillary pressure, residual trapping, and several other parameters of interest. While the wettability of CO2 on pure mineral and real rock sample have been studied a great deal over the past few years, two aspects of CO2 wetting have not been explored yet in detail: the first is the lack of understanding related to those processes that cause wetting shifts or aging on mineral surfaces over longer time scales as CO2 interacts with species in the brine and on the mineral surface. The second is the lack of understanding of how dynamic contact angles might evolve in real rock systems and how to relate static contact angle measurements to dynamic contact angle values. Several hypothesis were tested including (1) the ionic strength and valence of dissolved salts has an impact on contact angles; (2) the presence of organic species that are dissolved into solution and attached on mineral surfaces influences the wetting behavior; (3) dynamic flow results in different contact angle and could be correlated with capillary number, and (4) the interplay between solution chemistry and surface roughness determines the contact angle change.

To test these hypothesis, we carried out static captive bubble and dynamic contact angle measurements on polished mineral surfaces under high pressure and temperature conditions. Ionic strength and the valence of the dominant ions in the brine are found to have an important impact on static wettability which cannot be explained solely based on the shifts in the interfacial tension between the CO2 and brine. The effect of three organic species (formate, acetate, and oxalate) which are representative of species commonly encountered in the saline aquifers was explored. All three species show impacts on wettability, with the organics generally increasing the CO2 wetting of the mineral surface. This effect could be particularly important for organic rich repositories like depleted oil and gas fields or fractured shale formations where organic species could be presented both on mineral surfaces and in the aqueous phase.

To study the CO2-brine dynamic interactions we used two techniques to elicit movement of the contact line. In the first, a CO2 bubble is injected onto a surface and then retreated back to the injection port to elicit an adjective flow across the mineral surface. In the second, a CO2 bubble was placed in a vessel of brine not equilibrated with the brine and allowed to shrink and eventually disappear into the brine. These two methods lead to linear flow velocity range at the surface from millimeters per second to millimeters per day. The resulting contact angle changes were upscaled using capillary number, and a positive correlation was identified with capillary number. The interplay between surface roughness and solution chemistry determines dynamic contact angle, and the underlying mechanisms was identified as that the interaction of dissolved ions with surface charges on minerals only take effects when micron scale surface disparities are presented. These dynamic contact angle changes could help produce improved estimates of CO2 plume dynamics.

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Level-set simulation of capillary-controlled displacement on the pore scale with mixed wettability

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ABSTRACT

The distribution of fluids on the pore level in hydrocarbon reservoir rocks depends on the capillary pressure across interfaces and the wetting preference of the rock. These properties are required to assess methods for enhanced oil recovery (EOR) in the field, as they will affect the ability of the fluids to flow through the reservoir (i.e., relative permeability). Further, residual fluid saturations and the mechanisms for oil and gas trapping also depends on wettability. Thus, assessing the potential for CO2 storage by capillary trapping relies on understanding its relation to wettability. Since most hydrocarbon reservoirs displays a mixed-wet state, it is important to develop techniques that can simulate multiphase motion on the pore scale under mixed wettability conditions.

We have previously developed a level set method for simulating capillary-controlled two-phase displacements on the pore scale in porous media with arbitrary, yet uniform wettability [1]. The method uses a stepwise evolution velocity to distinguish capillary balance in the pore space from contact angle formation on the pore walls.

In this work, we adapt the level set method [1] to simulate capillary-controlled oil/water displacements at mixed wettability. We simulate drainage under water-wet conditions first, and establish mixed wettability on the pore level following [2], in which rock surfaces in contact with water remain water-wet, while all – or parts of – the other surfaces change to oil-wet. Before simulating imbibition, we implement an extension velocity step to propagate advancing contact angles defined on the pore walls in the normal direction into solid, which, in numerical tests, appears to be the most accurate method for describing contact angle when evolving the level sets using finite difference schemes with large numerical stencils to discretize gradients. To simulate water invasion, we add a water-wet and water-filled “porous plate” at inlet to prevent the water phase from leaving the domain.

We perform simulations on idealized, angular tubes with varying fractions of oil- and water-wet surface areas, and demonstrate that the simulated capillary entry pressures for water invasion agree with analytic solutions [3]. We also observe the different displacement regimes for varying wettability and initial saturations as predicted by analytic solutions [3], including (i) water invasion into the bulk of the pore with oil-layer formation, followed by oil-layer displacement (see attached figures), and (ii) water invasion without oil-layer formation. The method also describes correctly the pinning/de-pinning behavior of contact lines that separate surfaces of different wettability [4], as well as a correct transition between forced and spontaneous displacement during water invasion [3]. Finally, we present simulations (for a wide range of wettability conditions) that show how these

mechanisms change in real 3D geometries, such as in pore throats formed by the space between spherical grains, and in subsets of real rock geometries from micro-CT and FIB-SEM data sets. In all these simulation examples, we apply adaptive mesh refinement and demonstrate increased accuracy of our level set method for finer grids.

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Image-based modeling of single and two-phase flow in real rock

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ABSTRACT

The advantage of image-based direct numerical simulations (DNS) comprises the ability to model in detail dynamic physical fields interaction in “real” pore volume (and/or solid matrix) geometry. The models of this kind provide an access to abundant quantitative information and open a way to a powerful methodology combining the computer-assisted image generation, pore-scale simulations and dynamic visualization technique. However the future development of the methodology will inevitably encounter many obstacles.
To study the multiphase flow evolution in porous media (PM) the knowledge of instantaneous fluid distributions and interactions to solid grains and to each other is required. Rapidly advancing computed micro-tomography makes standard operation the generation of “real” PM images with typical resolution of few microns. At the same time the DNS experience of pore-scale flow remains relatively scarce and laborious due to the numerous practical challenges including typical model size, high computational expenses, uncertainties in geometrical description etc. Remind that the grain surface description is one of the important issues in pore-scale flow simulations, both single and multiphase.
Being one of the key subjects in pore-scale simulations the “real” pore/grain surface geometry adaptation for single (1P) and two-phase (2P) flow constitutes a main objective of our current work. X-ray micro-tomographic image based geometry built with pixels (2D) and voxels (cubes) has been used first without additional processing of grain surfaces. Diffuse interface approach combining Navier-Stokes and Cahn-Hilliard flow equations has been applied, which offers a framework dedicated to description of dynamic fluid interface.
Results on 1P and 2P flow in 2D synthetic geometry was first analyzed to quantify the effect of pixel size on absolute permeability and capillary imbibition dynamics. Different representation of the surface “rugosity” shape was used to illustrate its impact on the local velocity field. Both the grid discretization and the grain surface resolution (=pixel/voxel size) had the significant influence on 1P stationary flow and 2P dynamic capillary imbibition numerical results. In practice, the choice of numerical approach turned out to be not less important than above-mentioned factors.
It was expected that diffuse interface approach may offer a straightforward adaptation to voxel-based pore volume geometry starting from certain acceptable limit in voxel size. The acceptable voxel size can be medium-specific and defined according to required accuracy. Along with this the numerical analysis of capillary imbibition dynamics in “real” (Bentheimer) rock demonstrated that the image resolution and surface treatment are interrelated and should not be considered independently.

Numerical simulations of the Cahn–Hilliard equation in porous domains

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ABSTRACT

The Cahn–Hilliard equation is a well-known diffuse interface model for phase reordering in binary fluid systems. Our goal is to find a suitable discontinuous Galerkin method that is robust and computationally efficient on fine voxel-set-type grids arising from micro-CT imaging. We give an overview of possible time and space discretizations and propose a specific one. We discuss different derivations of modeling and controlling the equilibrium state contact angle of the diffuse interface touching the domain boundary. Optimal convergence against prescribed solutions is shown and robustness is demonstrated by various numerical scenarios.

Unconditionally stable methods for simulating two-phase multi-component interface models

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ABSTRACT

We consider multi-component dynamic two-phase interface models with Peng–Robinson equation of state. These models are derived from the minimum problems of Helmholtz free energy or grand potential in the realistic thermodynamic systems. The key challenges accoutered in numerical simulations are fully coupled relation and strongly nonlinearity. A linear transformation is introduced to decouple the relations between different components. From this, we further propose a semi-implicit time discretization scheme, which is unconditionally energy stable and solve the Cahn–Hilliard system by a decoupled way. Thus, our method can significantly reduce the computational cost and memory requirements. The mixed finite element methods are employed for the spatial discretization to guarantee the mass conservative property. Numerical results demonstrate the effectiveness of our proposed methods.

Evaluation Of Nanofluids for Oil Viscosity Reduction and Wettability Alteration in Heavy- oil Reservoirs.

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ABSTRACT

A new nanotechnology application was implemented in a set of wells of a Colombian field, located in the Llanos basin. Nanoparticles were engineered to reduce oil viscosity and to promote mobility in the near wellbore area in the reservoir, because of the wettability alteration. The understanding of physical and chemical processes taking place during injection/production periods is mandatory for lab test scale up and for a field-scale application as well. In this study, it is followed a coupled experimental-theoretical approximation for evaluating the new technology.
Initially the experimental tests was implemented with a flow assurance study followed a systematic approach, beginning with multiple compatibility test that were conducted with reservoir fluids for different operating conditions. Then, coreflooding tests evaluated the recovery factor and changes in petrophysical properties. Finally, lab test results showed that the nanofluids allows for a significant increment of the recovery factor. The application of the new technology in a series of pilot tests showed a significant impact on incremental production with an average increment about 30% for 6 months and the restauration of the original wettability from oil-wet to water wet.
From a theoretical approach, it was developed a conceptual model of the nanofluid based on physical & chemical phenomena of nanoparticles flooding into the reservoir. The mathematical model of the transport and retention of the nanoparticles in the reservoir considers the advective and diffusive transport of the nanoparticles in the oil phase. The nanoparticle model also accounts for their retention and further remobilization based on a two-step model. Transport and retention equations are coupled to a multiphase/multicomponent reservoir simulator. Besides, flow and transport equations are solved following the finite-volume method with a second-order discretization scheme.
The model predicts the evolution of nanoparticles distribution in the reservoir, in matrix and soluble phases as well, showing its effects on wells production. Labscale data were used to calibrate the parameters of the mathematical model. These model parameters were further upscales to reservoir conditions based on pilot test results.
The oil recovery factor can be estimated for a given well intervention using the novel mathematical model, which can be used for nanofluids deployment optimization procedures.

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Advances in modeling of enhanced oil recovery on general hexahedral grids

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ABSTRACT

Accurate numerical simulations are required for design and evaluation of enhanced oil recovery strategies such as nanoparticle, polymer and low salinity flooding. The mathematical models consist of a system of partial differential equations that are coupled, nonlinear, and possibly degenerate. There is a tight coupling of flow and transport in such problems and the flow parameters depend strongly on the transport solution. We have developed a Multipoint Flux Mixed Finite Element (MFMFE) method for the two-phase flow system in combination with an operator splitting algorithm for the reactive transport equations. Several solution schemes are presented, with varying degree of implicitness. Our approach provides a) computational efficiency of using general hexahedral geometry giving a high fidelity to the complex reservoir geometry, b) improved concentration and saturation front predictions owing to better calculation of advection, diffusion and dispersion terms, and c) reliable numerical schemes to solve the resulting system of reactive transport model.

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Multi-scale studies of the in situ remediation of chlorinated hydrocarbons by zero valent iron nanoparticles (nZVI) in porous media

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ABSTRACT

In spite of the great deal of work done for the in situ remediation of dissolved pollutants with nZVI [1], little progress has been made toward delivery of nZVI to NAPL source zones. The dechlorination rate is typically first order with respect to pollutant concentration, and hence the rate of DNAPL dechlorination can also be limited by the availability of dissolved contaminant [2]. This potentially limits the prospects of rapid and substantial DNAPL mass depletion [3]. Limited attention was paid on NAPL targeting by nZVI under flow-through conditions in real porous media [4]. Modeling 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 [5]. The objective of the present work is to identify the mechanisms and quantify the processes of bulk NAPL remediation when injecting nZVI suspensions in porous media polluted by chlorinated hydrocarbons.
For assessing the reactivity of aqueous suspensions of nZVI toward the dechlorination of tetra-chloro-ethylene (PCE), reaction tests are performed in batch reactors. To quantify the reaction kinetics, a shrinking-core-shell model is developed by accounting for the nanoparticle size distribution along with the mass-transfer and solid/liquid reaction mechanisms. For assessing the capacity of nZVI suspensions to dechlorinate the bulk phase of trapped PCE ganglia in porous media, nZVI injection experiments are performed on a glass-etched pore network and a soil column. The pore-scale visualization tests reveal that the gradual elimination of PCE ganglia by the injected nZVI is reflected in non-uniform interfacial configurations where the PCE ganglia are eroded in upstream regions dominated by high flow velocity (Fig.1). It is assumed that the overall process kinetics is controlled by two steps: (1) the enhanced PCE dissolution and (2) the reaction of dissolved PCE with the cores of ZVI nanoparticles. A macroscopic numerical model is developed where the nZVI injection in porous media is simulated as an advective- dispersive-reactive process by accounting for the nanoparticles attachment / detachment on pore-walls, and the kinetics of PCE dissolution and reaction is simulated with a true-to-the mechanism phenomenological model. The inverse modeling of experimental results enables us to estimate any unknown parameters of the investigated systems and evaluate the model predictability.

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Analytical Evaluation of Nanoparticles Utilization to Improve Injectivity in Porous Medium

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ABSTRACT

To deliver our understanding on nanoparticles utilization to remedy formation damage from in-house lab to field practice, this paper provides analytical solutions to explain how nanoparticles improve well injectivity. During re-injection of produced water or low salinity water flooding, the incompatibility between injected stream and reservoir fluids may lead to the detachment of fine particles, and thereby significant formation damage caused by particles plugging into pore-throats. Nanoparticles utilization has been reported widely to mitigate formation damage by controlling fines migration in the literatures. The aim of this paper is to develop fundamental theories and models to evaluate the enhanced injectivity by nanoparticles usage to guide oilfield nanoparticles applications.

In this paper, the positive contribution of nanoparticles to mitigate particles migration is characterized by the increase of maximum retention concentration of particles on rock grains via reducing the surface potential between rock grains and particles. We develop semi-analytic MOC solutions for two different scenarios of nanoparticles utilization to control fines migration: (1) co-injection of nanoparticles with fines suspension into one-dimensional permeable medium and (2) pre-coating porous medium with nanoparticles before fines injection to evaluate the enhanced capability of porous medium to capture unsettled fines by success of nanoparticles utilization. In addition, other two reference scenarios with nanoparticles usage are presented to distinguish the merits of nanoparticles. The suspended, attached, and strained particles concentration profile and effluent particles concentration history are used to compare and confirm the success of nanoparticles treatment. The improved well injectivity by nanofluid injection is presented as an explicit formulation of injectivity index.

It turns out that (under certain conditions) the analytical solutions may contain nanoparticle adsorption front, suspended fines front, and attached fines front appearing as weak discontinuities. The mitigation index (MI) is defined to evaluate the success of nanoparticles to control fines migration. This paper also provides a flowchart to how to explain lab experiments or filed examples. In addition, the proposed approach provides a fast and reliable method to optimize nanoparticles treatment (nanoparticles concentration and the required amount) to control fines migration.

Through quantitative comparison of effluent particulates concentration and permeability decline history, we apply lab experimental findings to verify the accuracy of analytical solutions. In practice, our analytical approach provides valuable insights into how nanoparticles utilization can help reduce fines migration in types of reservoirs suffering from fines migration problems.

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Numerical Investigation of Nanofluid Evaporation Flow through Porous Wick

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ABSTRACT

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Key Words: heat pipes, wick structure, evaporation, thermal performance

Abstract
Increase in compactness in electronic equipment, the heat generation rate through these components increase with a large amount. To maintain the electronic components in their operating temperature range various cooling devices are used to dissipate heat from these electronic components. Heat pipes are widely used in electronic cooling because of its ability to transport heat without any external pumping devices and the heat transfer phenomena involves phase change nearly in isothermal condition. Our present study is concentrated on the phenomena of phase change when the working fluid flows through the wick in the evaporator section of heat pipe. Evaporation in heat pipe is largely influenced by the structure of the porous media a good understanding of porous media property is necessary to increase the thermal performance of heat pipes. In this study numerical simulation of nanofluid evaporation through porous wick is done in fluent. A two dimensional rectangular porous structure is used with different values of porosity and permeability value. Reynolds number of flow is calculated to know the nature of the flow, a volume of fluid multiphase model is used to track the two phases; Aluminium oxide+water is used as a working fluid in our analysis. Simulation is performed in unsteady state condition. Capillary pressure, vapor mass fraction, mixture temperature are computed for different values of porosity and permeability value. Based on the results obtained thermal performance of heat pipes with different porous media properties have been compared.

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Nanoparticles Adsorption/Detachment and Its Effects on Permeability of Water-wet Berea Cores: Experiments and Modeling

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ABSTRACT

Recently, nanoparticle application has been widely reported in diverse potential applications in the oil and gas industry, including formation damage mitigation, assisted surfactant/alkaline/low salinity/gas flooding, and well treatment after fracturing in unconventional reservoirs et al. However, when nanoparticles without enough dispersant stability pass through pore throats, they can be adsorbed and plugged in pore-throats to cause permeability impairment. The aim of this paper is to present both experimental and mathematical investigations on nanofluid flow with dynamic adsorption/detachment behavior and its negative effects on formation permeability, and to provide insights to the importance of nanoparticles design before application.

In this paper, we conduct core-flooding experiments on water-wet Berea sandstone to evaluate nanoparticles adsorption behavior and formation permeability by observing the displacement pressure gradient and effluent nanoparticles concentration. Two typical nanoparticles, hydrophilic nano-structure (NSP) and colloidal nanoparticle (CNP), are dispersed in the injected brine stream at 0.05, 0.2 and 0.5wt% concentrations. During the core-flooding process, the corresponding pressure drop across the cores is recorded to estimate nanoparticles adsorption and retention behavior, as well as particles detachment during brine post-flush. Nanoparticle concentration profile along the core plug and the propagation of adsorption front are evaluated to match the metrical outlet concentration. In order to quantify nanoparticles adsorption and its effects on fluid flow, an analytical model is also derived using method of characteristics to characterize the complex nanoparticles adsorption, straining and detachment behaviors and their associated formation damage effects. The interplay between nanoparticles and rocks is described by a physical-chemical reaction model

The experimental results indicate that both adsorption and detachment occur during the injection process. The extent of adsorption and retention for nano-structure particles (NSP) is high by recording rapid increase of pressure drop, while colloidal nanoparticles (CNP) does not adsorb or retain too much. Nanoparticle injection concentrations and sizes are also critical to control particles adsorption/detachment behavior. The optimal silica nanoparticles is found as colloidal nanoparticle (CNP) with customized 18nm particle size, which almost bring no negative effects the permeability of water wet cores. In addition, the analytical solutions showed a good agreement with the experimental results.

In practice, this paper has the following contribution, 1) apply lab experiments to highlight the importance of optimal nanoparticles design to enhance oil/gas recovery application. 2) The analytical solution provides physical insights to evaluate nanofluid flow performance with adsorption/detachment.

dynamic reconstruction of porous materials and microstructure evolution

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ABSTRACT

Reconstructing heterogeneous materials from limited structural information has been a topic that attracts extensive research efforts and still poses many challenges. The Yeong-Torquato[1] procedure is one of the most popular reconstruction techniques, in which the material reconstruction problem based on a set of spatial correlation functions is formulated as a constrained energy minimization (optimization) problem and solved using simulated annealing. The standard two-point correlation function S2 has been widely used in reconstructions, but can also lead to large structural degeneracy for certain nearly percolating systems[2]. To improve reconstruction accuracy and reduce structural degeneracy, one can successively incorporate additional morphological information (e.g., nonconventional or higher-order correlation functions), which amounts to reshaping the energy landscape to create a deep (local) energy minimum. In this paper, we present a dynamic reconstruction procedure that allows one to use a series of auxiliary S2 to achieve the same level of accuracy as those incorporating additional nonconventional correlation functions. In particular, instead of randomly sampling the microstructure space as in the simulated annealing scheme, our procedure utilizes a series of auxiliary microstructures that mimic a physical structural evolution process (e.g., grain growth). This amounts to constructing a series auxiliary energy landscapes that bias the convergence of the reconstruction to a favored (local) energy minimum. Moreover, our dynamic procedure can be naturally applied to reconstruct an actual microstructure evolution process. In contrast to commonly used evolution reconstruction approaches that separately generate individual static configurations, our procedure continuously evolves a single microstructure according to a time-dependent correlation function. The utility of our procedure is illustrated by successfully reconstructing nearly percolating hard-sphere packings and particle-reinforced composites as well as the coarsening process in a binary metallic alloy.

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Reconstruction of disordered porous materials and media

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ABSTRACT

Porous media and materials are ubiquitous and have a wide variety of applications. Having an accurate model of porous media is critical to the evaluation of physical properties of such media and materials. Hence, accurate modeling of porous media and materials has been a highly important that has been studied for decades. An impediment to accurate modeling of porous media is the fact that heterogeneity is one of their distinct characteristics, and the question of how to incorporate it in a model meaningfully is still an open question. Several methodologies have been presented to better represent the variability and complexity in porous media. Among them is a class of methods that are based on some object and/or process-based techniques. They are not, however, not sufficiently accurate to capture the heterogeneity and complexity of porous media, particularly the natural ones. On the other hand, stochastic statistical-based methods can be used when either little or no information is available. In this paper, a recent reconstruction approach, called cross-correlation based simulation (CCSIM), is presented in which an initial set of training data (such as an image) is used to directly convey the morphology of the pore space. The CCSIM algorithm can be used for direct 2D to 2D, 3D to 3D and 2D to 3D reconstruction. Furthermore, one can also use the method for reconstruction of non-stationary porous media, a notoriously difficult and unsolved problem. The application of the technique for the important problem of reconstruction of 3D porous media using a single 2D thin section, proposed by the authors for the first time, is demonstrated for various types of porous media. The method provides high quality realizations of porous media in a matter of a few CPU seconds.

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Research on 3D digital core reconstruction algorithm

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ABSTRACT

One of the main research areas of our research group is the digital core 3D reconstruction using one single 2D training image. There are two most commonly adopted reconstruction algorithms in this area: Simulated annealing algorithm whose target is statistical function-matching and Multiple-point statistics (MPS) algorithm whose target is pattern-matching. The main research achievements we have made on these two algorithms are as follows:

1. Simulated annealing algorithm

(1) Reconstruction of multiphase microstructure

The SA methodology can be used to reconstruct the 3D microstructure of multiphase sandstone from limited morphological information of the 2D microstructure. This methodology utilizes the two-point correlation function and LPF as morphological descriptors to reproduce the microstructure. Though it is difficult to reconstruct the three-phase microstructure, the reconstruction of the three phase microstructure has the following advantages: it not only provides an accurate 3D microstructure showing the space distribution of different phases but it mainly helps us to analyze the effect of different phases on the macroscopic properties.

(2)Stable-phase method for hierarchical annealing

A stable-phase method for hierarchical annealing can solve the high demand for computational resources associated with simulated annealing for the reconstruction of large-scale binary porous media images. The most significant advantage of our presented model is the reduction in the number of exchanged pixels by the annealer in the overall hierarchy. In our method, only 5.21% of the pixels in the overall hierarchy need to be considered for sampling by the annealer: an order of magnitude reduction in the computational requirements.

2. Multiple-point statistics (MPS) algorithm

A random three-dimensional (3D) porous medium can be reconstructed from a two-dimensional (2D) image by reconstructing an image from the original 2D image, and then repeatedly using the result to reconstruct the next 2D image. The reconstructed images are then stacked together to generate the entire reconstructed 3D porous medium. To perform this successfully, a very important issue must addressed, i.e., controlling the continuity and variability among adjacent layers. Continuity and variability, which are consistent with the statistics characteristic of training image (TI), ensure that the reconstructed result matches the TI. By selecting the number and location of the sampling points in the sampling process, the continuity and variability can be controlled directly, and thus, the characteristics

of the reconstructed image can be controlled indirectly. In our research, we propose and develop an original sampling method called three-step sampling. The continuity and variability of adjacent layers were considered during the three steps of the sampling process.
We focus on the methods including CCSIM proposed by Tahmasebi and Hajizadeh, SIMPAT proposed by Arpat and Caers, and SNESIM proposed by Strebelle. Certainly we also pay attention to other methods, such as Texture synthesis, Markov random fields, fast frequency-domain transformation, discrete wavelet transformation algorithms, and neural network algorithms.

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Multiscale Characterization of Pore Structures in Geological Materials: Combination of Small- and Ultra-small Angle Neutron and X-ray Scattering with Imaging Results

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ABSTRACT

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. In order to interpret the history of any geological system, the physical and chemical “fingerprints” of this evolution must be fully explored over widely different length scales from the nanoscale to the macroscale.

It is, however difficult to completely describe textural and porosity changes in rock samples using direct imaging techniques alone because of the wide variation in length scales involved. Depending on the sample porous spaces in geological materials range in scale from a few Ångstroms to many meters. Even if only hand-sample (core) sized materials are considered, porosity frequently ranges over at least seven orders of magnitude (nm – cm). X-ray and electron imaging approaches (XCT, SEM, TEM) tend to be limited either in resolution or, at high magnifications, in an ability to present a statistically meaningful description of the pores structure.

These limitations can be overcome, however, by combining imaging results with those from small and ultra-small angle neutron and X-ray scattering ((U)SANS and (U)SAXS). Scattering contrast in rock samples arises primarily from the difference in the scattering length densities of the rock and the pores within it. Because the scattering cross-section is proportional to the Fourier transform of the geometric correlation function imaging and scattering data can be combined to provide a multiscale quantification of pore structures, including data on overall porosity, pore volume distributions, connectivity (effective porosity), and surface and mass-fractal behavior. Both overall averaged values, as well as mapping of multiscale porosity at submillimeter resolution are possible. This talk will describe the connection between imaging and scattering approaches, and provide examples of our work in this area (cf. Anovitz et al., 2009, 2013, 2015a,b; Anovitz and Cole, 2015) in both geological, and rock-like (cement) materials.

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Morphological modelling of the capillary condensation and evaporation isotherm of porous media

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ABSTRACT

A method based on morphological operators is proposed to numerically simulate the capillary condensation and evaporation isotherm of digital porous media. Instead of iteratively updating the liquid-vapor interface as in Štepánek et al. (2007), the method extends the analysis of Münch and Holzer (2008) who simulated mercury intrusion porosimetry from FIB-nanotomography.

In the present work, the equilibrium states of the Kelvin equation are used to numerically predict the menisci of the vapor-liquid interface which depends on the pressure and local pore geometry. Liquid condensation during absorption is simulated using a morphological closing operator. The diameter of the spherical structuring element controls the radius of curvature of the vapor-liquid interface. A combination of closing and hole-filling operators is used to simulate desorption. The method allows one to predict the hysteresis and pore size distribution associated to absorption and desorption porosimetry curves on simple geometry as well as complex random media.

The numerical algorithm is first validated using simple configurations made of e.g. an "ink-bottle" pore or a union of cylindrical and spherical pores. The resulting isotherms compare well to theoretical expectations. Second, the method is applied to a variety of random porous media, making use of representative volume elements. For random media, strong finite-size effects are observed for the desorption curves. This problem is solved by taking into account vapor percolation during the simulation. Boolean random media with spherical and cylindrical primary grains are then considered, for the porous or solid phases. The effect of the grains elongation is assessed. Third, the hysteresis associated to several Boolean models of multi-scale materials are investigated and discussed.

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CHEMICAL DEGRADATION OF A NUMERICAL MATERIAL – APPLICATION TO FONTAINEBLEAU SANDSTONE

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ABSTRACT

The carbon capture and storage consists in injecting large quantities of CO2 in supercritical form directly into deeply located geological formations. During the geological storage, chemical reactions may induce some important and irreversible changes of the rock properties [1].
The morphology of the pore network and solid skeleton defines important macroscopic properties of the rock (permeability, stiffness). The proposed micromechanical approach is based on the following morphological criteria [2]:
— basic measures: volume fraction, surface areas of phases
— sizing: distributions of pores or grains size
— spatial distribution: estimation of characteristic length scale, geometrical dispersion, anisotropy
— connectivity: which highly influence on permeability (existence of percolation)
Sandstones are products of a series of complex geological and hydrodynamical processes. In simplified way it can be described by sandgrains transport, deposit, compaction and diagenesis. In this work we reconstructed the 3D sandstone geometry by simulating the way of the sandstone-forming processes. The reconstruction method consists of three main steps [3]:
— sedimentation: grain deposit
— compaction: bulk volume reduction and pore space extension
— diagenesis: decrease of the characteristic size of the porous phase.
Generated samples satisfy aforementioned morphological and statistical informations which were obtained by 3D image analysis of X-ray tomography of the natural rock sample [Fig. 1 and Fig. 2].
The chemical degradation of the material is taken into account by performing the numerical erosion of the microstructure by using 26-neighbourhood structuring element. We proposed two scenarii of numerical dissolution:
— the first scenario (isotropic dissolution): consists in dissolving all the pore space
— the second scenario: consists in dissolving only percolated porous network.
The proposed modelling is universal in the sense that it uses non-dimensional time scale that can be adjusted to a particular time-dependent process.
Some numerical upscaling techniques (linear homogenization, effective Darcy's law) are used in order to estimate evolution of elastic effective behaviour and permeability, triggered by progressive dissolution of microstructure. A new methodology enabling imposing periodic boundary conditions, in order to estimate mechanical properties, on non-periodic geometry is proposed. A link between effective elastic moduli and permeability is proposed [Fig. 3].

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Toward Simplified description of Reservoirs Using Quasi Steady State Storativity and Connectivity Matrix of Wells in 3D Heterogeneous Formations

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ABSTRACT

Increasing complexity of hydrocarbon recovery in natural reservoirs needs a careful well pattern development. Modern drilling techniques add extra freedom in the well pattern architecture. In order to help finding the best well architecture, and also to set up the best secondary recovery scheme, it is appealing to be able to build a simple model summarizing the interwell connectivities and the associated drainage area of each well, before processing expensive detailed multiphase reservoir simulations. This is the goal of the presentation.
In single phase conditions, using the linearity of the underlying equations, and a quasi steady state hypothesis, it is shown that the simplest model is a set of first-order linear differential equations relating each pressure variation at each well to its time derivative and the fluid rate. This introduces the so-called storativity
matrix and a transmissivity matrix that summarize the coupling of the wells with the geological formation and between themselves. It is shown in a rigorous manner that the transmissivity and storativity matrices are directly related to base solutions o the Laplace equation to be solved over the whole reservoir domain with appropriate boundary conditions. Explicit formulae are given, allowing one to use existing reservoir simulators to compute both matrices. An analogy with upscaling approaches is done. The sensitivity of the transmissivity matrix to internal heterogeneities of the reservoir is also provided. It is shown that this evaluation has a negligible extra cost, which permits to set up matching loops allowing to match field data and detailed reservoir models.

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Generalized Multiscale Finite Element Methods for problems in perforated domains

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ABSTRACT

In this work we develop a generalized multiscale finite element methods (GMsFEM) for problems in perforated domains. The problems in perforated domains are of great interest for many applications. The main characteristics of these problems is that the underlying processes occur in multiscale domains where the geometry of the domain has multiple scales, e.g., domain outside inclusions. There are many important applications for processes in perforated domains. For example, fluid flow in porous media, diffusion in perforated domains, mechanical processes in hollow materials, and so on.
The problems in perforated domains are of multiscale nature. The solution techniques for these problems require high resolution. In particular, the discretization needs to honor the irregular boundaries of perforations. This gives rise to a fine-scale problems with many degrees of freedom which can be very expensive to solve.
We investigate multiscale approaches that attempt to solve such problems on a coarse grid by constructing offline and online multiscale basis functions in each coarse grid, where the coarse grid can contain many perforations. In particular, we are interested in cases when there is no scale separation and the perforations can have different sizes [1,2,5]. In our work, we follow Generalized Multiscale Finite Element Method (GMsFEM) and develop a multiscale procedure where we identify multiscale basis functions in each coarse block using snapshot space and local spectral problems [3-6].
In the work, we consider commonly used model problems including the Laplace equation, the elasticity equation, and the Stokes system in perforated regions. Our approaches start with the offline procedure, which constructs multiscale basis functions in each coarse region and formulates coarse-grid equations. We present an online procedure, which allows adaptively incorporating global information. We present online adaptive enrichment algorithms for the three model problems mentioned above. To illustrate the performance of our method, we present numerical results with both small and large perforations.

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Multiscale Local Orthogonal Decomposition and Applications to Heterogeneous Media

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ABSTRACT

Multiscale methods often depend on periodic microstructures to arrive at error estimates. This limits the robustness and confidence in simulations when general heterogenous coefficients are considered. With the local orthogonal decomposition (LOD) method, we are able to create an efficient multiscale method that has precise error estimates with minimal regularity on the coefficients. The method relies on the frameworks of Variational Multiscale Methods. By using a dual grid framework, and using quasi-interpolation operators on the coarse grids we are able to define a fine-scale space. This is accomplished by taking the kernel of the quasi-interpolation operators on this coarse grid to be a fine-scale space. With this fine-scale space, we solve correction problems at each node in the coarse grid, and correct the coarse-grid approximation space with the fine-scale space details from these solves. This new space is the so-called multiscale approximation. These multiscale approximations yield optimal approximations independent of oscillations, however, the corrections are global and must be truncated. Using local truncations, we are able to calculate the order of error as a function of the truncation patch size.

In this talk, we discuss some current developments in extending the LOD method to applications with microstructure and the elimination of pollution in heterogenous Helmholtz propagation. The main challenges in these application is in the analysis of geometric parameters in the case of complicated microstructure. In the case of Helmholtz is the analysis of frequency dependent stability estimates. We report some of the current state-of-the-art estimates in the case of frequency stability in heterogenous Helmholtz equations.

Multiscale modeling for reservoir geomechanics

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ABSTRACT

The demand for accurate and efficient simulation of geomechanical effects is widely increasing in the geoscience community. The mathematical formulation that describes deformation of a geological formation coupled with flow and transport entails heterogeneous coefficients with a wide range of length scales. Such detailed descriptions of hydro-mechanical properties impose severe computational challenges and motivate the development of multiscale solution strategies.

In the present work we extend the multiscale solution framework presented in [1,2] to the simulation of the mechanical response of heterogeneous geological porous media. Constructed on finite element fine-scale system, we show that the framework developed for flow through porous media can be quite naturally generalized to the geomechanical equilibrium problem. After imposing a coarse-scale grid, the construction of the coarse scale basis functions is performed solving local equilibrium problems within coarse cells. Such basis functions form the restriction and prolongation operators used to obtain the coarse-scale systems for the displacement. Then, a two-stage preconditioner, that couples the multiscale system with a local smoother, is derived for the iterative solution of the fine-scale linear system. Numerical experiments are presented to illustrate the accuracy and robustness of the method with respect to distorted mesh, material anisotropy and boundary/loading conditions.

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Non-local formulation for multiscale flow in porous media

Presenter: Amir Hossein Delgoshaie
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ABSTRACT

The multiscale nature of geological formations is reflected in the flow and transport behaviors of the pore fluids. For example, multiple pathways between different locations in the porous medium are usually present. The length, and strength of these flow paths can vary significantly, and the total flow at a given location can be the result of contributions from a wide range of pathways between the points of interest. A single continuum model can capture the contributions from all the flow paths correctly only if the chosen computational cells are much larger than the longest pathway. However, depending on the densities and lengths of these long pathways, choosing the appropriate size of the control volume that allows for a single continuum description of the properties, such as conductivity, may conflict with the desired resolution for the flow field.

To capture the effects of the multiscale pathways on the flow, a non-local continuum model is described. The model can represent non-local effects, for which Darcy's law is not valid. In the limit where the longest connections are much smaller than the size of the control volume, the model is consistent with Darcy's law. The non-local model is used to describe the flow in complex pore networks. The pressure distributions obtained from the non-local model are compared with pore-network flow simulations, and the results are in excellent agreement. Importantly, such multiscale flow behaviors cannot be represented using the local Darcy formulation.

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Reduced order modeling of nonlinear electrokinetic transports in porous structures

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ABSTRACT

The current study is focused on the numerical modeling of fluid and ion transports through porous structures exposed to external gradients of pressure, electric potential, and concentration. The pores in these networks are typically charged on the surfaces when filled with fluid electrolytes. The surface charge attracts equal amount of counter-ions from the bulk solution to regions close to the pore walls. The thickness of this charged region is characterized by the Electric Double Layer (EDL). Due to the presence of EDLs in such systems transport of ions and fluid are coupled via electrostatic interactions leading to wide range of phenomena such as electroosmosis, diffusion-osmosis, and streaming current. Additionally, the exchange of ions between bulk and EDL within each pore can lead to nonlinearities such as concentration polarization shocks [1,2] and a mechanism for overlimiting current in confined structures [3]. Furthermore, in a network of pores with pore-size variations, the interactions between various modes of transport may provoke additional complexities, such as internal flows and mixing. The described effects play important roles in the systems relevant to various technological applications including supercapacitors for energy storage [4], deionization and purification systems [5], and lab-on-a-chip devices [6].

We have developed and validated a computationally efficient model to study the nonlinear ion transport through electrokinetic porous structures. This approach bridges the gap between traditional homogenization methods, which fail to capture the pore-scale nonlinearities [7], and expensive direct numerical simulations (DNS), which have to resolve complex geometries in multi-dimensions. We use coupled Poisson-Nernst-Planck-Stokes equations to mathematically describe the underlying physics of the problem. We assume that a porous medium is a network of long and thin (low aspect ratio) pores. Physically, this implies that the transport is quickly equilibrated in the thin dimensions representing pore cross-sections. Thus, the full three-dimensional equations are simplified into two sets of reduced models: (1) equilibrium equations in the thin dimensions, and (2) area integrated transport equations in the longitudinal direction of pores. The second set relates the area-integrated fluxes including fluid flow, electric current, and ion transport to the local gradients of pressure, potential, and concentrations. The pre-factors of gradient terms are area-averaged quantities depending on the solutions of equilibrium equations, which are parameterized by the local pore electro-chemical properties. These solutions are obtained for a wide range of controlling parameters and tabulated in the form of area-averaged transport coefficients. We have developed a fully conservative numerical implementation of such model with no limitation on the thickness of EDL. This model is able to simulate general networks of low aspect ratio pores with significantly lower computational cost compared to DNS, and can accurately capture the nonlinear response of the system. We will demonstrate example calculations highlighting validation of this model as well as simulations of random networks.

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Vertically-integrated dual-porosity models for CO2 injection and migration in fractured reservoirs

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ABSTRACT

Geologic carbon dioxide (CO2) sequestration is a promising carbon mitigation technology to reduce anthropogenic CO2 emissions into the atmosphere. To safely store large amounts of CO2 in the deep subsurface, computationally efficient mathematical models are essential to accurately predict CO2 and brine migration. One type of simplified model can be developed by integrating the three-dimensional governing equations in the vertical dimension. The dimension reduction resulting from vertical integration leads to a very computationally efficient model; we refer to these as vertically-integrated models. In the past decade, a range of vertically-integrated models with different levels of complexity have been developed and applied to field-scale modeling of CO2 injection, migration and leakage. Almost all of them have been based on the assumption of vertical equilibrium for the two fluid phases. One recent exception to this is the work of Guo et al. (2014) that introduced the concept of dynamic reconstruction to include vertical dynamics within vertically-integrated models.

To date, vertically-integrated models have not been developed for CO2 and brine migration in fractured reservoirs. CO2 injection into a fractured reservoir involves two different characteristic time scales, one for buoyant segregation in the fractures and a second for the fluid dynamics in the matrix. The high permeability of the fractures leads to fast buoyant segregation of CO2 and brine in the vertical direction within the fractures, and therefore the vertical equilibrium model may be applicable. The flow in the matrix is much slower and involves longer time scales for segregation; thus the vertical equilibrium approach may not apply.

In this paper, we treat the fractured reservoir as a dual continuum and develop a hybrid vertically-integrated framework, with different vertically-integrated models used in the fracture and the matrix, honoring the different buoyant segregation time scales. We use a vertical equilibrium model for the fracture domain and explore different model options for the matrix domain, including a dual-porosity model and other models that involve non-equilibrium reconstructions of CO2 and brine in the vertical direction within the context of a vertically integrated model. A corresponding vertically-integrated mass transfer function is derived and used to model the mass exchange between the fracture and the matrix domains. We adopt different mass transfer functions, taken from the literature, and compare results from this hybrid model with a full-multidimensional model in terms of model accuracy and computational efficiency. Finally, we apply the hybrid model to a fractured reservoir for CO2 migration and investigate storage capacity and trapping efficiency.

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Some multiscale model reduction methods and their applications for flows in random porous media

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ABSTRACT

Stochastic modeling has become a popular approach to quantify uncertainty in multiscale models. The uncertainty in multiscale structure properties is often parameterized by a high-dimensional random variable. This leads to a deterministic problem in a high-dimensional parameter space and the numerical computation becomes very challengeable as the dimension of the parameter space increases. To efficiently tackle the high-dimensionality, we present some dimension reduction techniques, through which the high-dimensional stochastic model is decomposed into some lower-dimensional models. To treat the multiscale properties, numerical multiscale methods are used to simulate each of derived stochastic models. The synergy of the stochastic dimension reduction techniques and the multiscale methods reduces the stochastic multiscale models in both stochastic space and physical space, and significantly decreases the computation complexity. The presented multiscale model reduction methodology is applied to flows in random porous media.

An Efficient Multiscale Mixed Finite Element Method for Modeling Flow in Discrete Fractured Reservoirs

Presenter: Zhaoqin Huang
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ABSTRACT

Fractures can significantly impact the flow patterns of carbonate reservoirs and should be accurately accounted for in a geological model. Accurate modeling of flow in fractured media is usually done by discrete fracture model (DFM), as it provides a detailed representation of flow characteristic. However, DFM poses a particular challenge to traditional numerical method with regard to computational efficiency and accuracy. In this study, a multiscale mixed finite element method (MsMFEM) has been proposed for detailed modeling of two-phase oil-water flow in fractured reservoirs. The MsMFEM uses a standard Darcy model to approximate pressure and fluxes on a coarse grid. Fine-scale effects of fractured media are captured through basis functions constructed numerically by solving local DFM on the fine-scale grid. In our approach, we consider arbitrary fracture orientations and use triangular fine grid. Through multiscale basis functions, we can maintain the efficiency of an upscaling technology, while at the same time generate a more accurate and conservative velocity field on the full fine-scale grid. Comparisons of the multiscale solutions to the fine-scale discrete fracture model solutions indicate that the fine-scale flow in fracture networks can be represented within a coarse-scale Darcy flow model. The results demonstrate that the MsMFE technology is a promising method toward fine flow simulation of high-resolution geological models of fractured reservoirs.

Algebraic Dynamic Multilevel Multiscale (ADM) Fully Implicit Method for Multiphase Flow in Heterogeneous Porous Media

Presenter: Matteo Cusini
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ABSTRACT

A novel algebraic dynamic multilevel multiscale method (ADM) is developed for fully implicit (FIM) simulations of multiphase flow in homogeneous and heterogeneous porous media. The PDEs describing the multiphase displacement are first obtained using FIM (fully-coupled simultaneous) method on a high-resolution fine-scale grid, honoring the heterogeneous geological properties. Built on this FIM system, ADM constructs a space-time adaptive multiscale FIM system on a dynamically defined multilevel nested grid. The grid resolution is automatically defined on the basis of an error estimate criterion, aiming to minimize the accuracy-cost trade-off. The ADM system is algebraically described by employing sequences of adaptive multilevel restriction and prolongation operators. Restriction operators are constructed using a finite volume scheme, so that mass conservation of the solution on the dynamic grid is ensured. This allows for better stability and accuracy of the multiphase transport simulations. Different choices for prolongation operators are considered, namely, constant, bilinear and multiscale basis functions. By construction, all of them ensure partition of unity. For several homogeneous and heterogeneous test cases, it is illustrated that ADM employs only a fraction of the total number of fine-scale grid cells in order to provide accurate solutions. The sensitivity of the ADM solutions to the number of employed multilevel grid cells and the error threshold value is investigated in detail. ADM is an important advancement of mulsticale methods for fully implicit simulations because it solves for both pressure and saturation unknowns simultaneously (FIM) on an adaptive multilevel grid. At the same time, it is a significant step forward in the application of dynamic local grid refinement techniques for heterogeneous formations. More precisely, ADM provides multilevel quantities while honoring the fine-scale heterogeneous coefficients, and it does not rely on homogenized or upscaled coarse-scale quantities. Finally, its algebraic formulation allows for convenient integration with existing advanced simulation platforms. As such, ADM is an important advancement for next-generation reservoir simulators.

Applicability conditions for model-order reduction of reactive transport in bi-disperse porous media

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ABSTRACT

We investigate the applicability conditions for sequential model-order reduction of reactive solute transport in bi-disperse porous media, where the reduction is performed through the method of homogenization. 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 [1], 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.
At the pore-scale we consider the Stokes and the advection-diffusion equations to model flow and transport, respectively. The surface reaction enters as a boundary condition in the transport equation. In the first step of sequential homogenization, the "closure problem" [2] is solved for both flow and transport at the pore-scale. As a result, we determine the effective permeability and the dispersion tensor. In the second step, we solve a "closure problem" for the meso-scale scale using effective media parameters from the pore-scale. We compare the sequential upscaling results with the direct solution of the fully resolved pore-scale problem. The convergence rate of the sequential "closure problem" requires that pore-scale has to be separated enough with the meso-scale. Finally, we compare the direct pore-scale simulations with the homogenized model and show that reaction rates at each level should satisfy the applicability regimes identified by Battiato & Tartakovsky [3]. The cell-averaged numerical solution was reconstructed by first order conservative total variation diminishing (TVD) reconstruction scheme from the finite volume (FV) methods.

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Multiscale Numerical Methods For Solving Nonlinear Forchheimer Equation in Highly Heterogeneous Porous Media

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ABSTRACT

In this talk, I will present a local multiscale model reduction for nonlinear flows in heterogeneous porous media. I will consider generalized Forchheimer equations. The generalized Forchheimer equation describes flows at Darcy scales and arises when the pore-scale velocity is large. We consider the two term law form of Forchheimer equation and write the resulting system in terms of a degenerate nonlinear flow equation for the pressure. Our multiscale model reduction can be considered a generalization of recently introduced upscaling and numerical homogenization techniques, where the authors consider problems with scale separation. In the proposed approach, we construct local reduced-order model by constructing appropriate snapshot spaces and local spectral problems within the framework of Generalized Multiscale Finite Element Method (GMsFEM). To save the computational time, we use empirical interpolation techniques in estimating the nonlinear terms. I will discuss the use of adaptive procedures both in offline and online stages of the computation. We present numerical and theoretical results for the proposed method.

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Least-Squares mixed generalized multiscale finite element method for flow problems in porous media

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ABSTRACT

In the poster, a least-squares mixed generalized multiscale finite element method (GMsFEM) is proposed to solve flow problems in highly heterogeneous porous media. The goal is to construct multiscale basis functions for both pressure and velocity simultaneously. We will apply the framework of GMsFEM, and design systematic strategies for the construction of basis. The problem is formulated in a least-squares mixed form, for which compatibility condition for the pressure and velocity spaces is not required. This significantly enhances the flexibility to choose multiscale basis functions. A flux correction technique is developed to obtain the velocity with local mass conservation. The method can give accurate solutions for both pressure and velocity with the use of only a few basis functions per coarse element. Convergence results will be presented. Some numerical examples will illustrate the performance of the least-squares mixed GMsFEM.

Selection of representative realizations for optimization under geological uncertainty

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ABSTRACT

In the robust optimization of oil/gas reservoir performance, decision parameters (well locations, flowrate/pressure settings) are often determined by maximizing the expected value of an economic objective over a set of geological realizations. These realizations are intended to capture the current state of knowledge regarding subsurface geology. Each iteration of the optimization algorithm requires performing a flow simulation for every realization considered. Because computational cost scales directly with the number of realizations employed, it is preferable to use as few realizations as possible. If too few realizations are considered, however, results may be suboptimal because geological uncertainty is not properly represented. In order to achieve the optimal balance between cost and representivity, the set of geological realizations must be selected very carefully.

In this talk, we introduce a new approach, based on clustering, for the selection of representative sets of realizations. Prior to clustering, each realization is represented by a low-dimensional feature vector that contains a combination of permeability-based and flow-based quantities. Calculation of flow-based features requires the specification of one or more flow problems, which we choose to be consistent with the specifications and constraints in the target optimization problem. Permeability information is captured in a reduced form through use of principal component analysis.

We consider the impact of different weightings for flow and permeability information in the clustering. Several treatments are first tested for random well configurations and settings, as are encountered during optimization when stochastic search algorithms are applied. If we designate f_sub as the expected flow response vector computed using the selected subset of realizations, and f_full as the expected response vector computed for the full set of realizations, the goal is to find the weights in the clustering that lead to realizations that provide an f_sub that is closest to f_full (for a given number of selected realizations). From detailed tests for two example cases, we find that permeability-based clustering is generally preferable for representing the expected flow response for (new) random multiwell configurations. Clustering that includes flow information is, however, the better option for capturing the expected flow response for random well settings (wellbore pressures in this case).

The various procedures are then used to select realizations for optimization under uncertainty. Separate optimizations of multiwell configurations and well settings are considered. We show that optimization results are generally consistent with the findings for random configurations and settings. This suggests that our framework should be applicable for a range of problems involving optimization of subsurface operations under geological uncertainty.

A fast distribution method for complex nonlinear two-phase flow in complex stochastic porous media

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ABSTRACT

Because geophysical data are inexorably sparse and incomplete, stochastic treatments of simulated responses are convenient to explore possible scenarios and assess risks in subsurface problems. In particular, understanding how uncertainties propagate in porous media with nonlinear two-phase flow is essential, yet challenging, in reservoir simulation and hydrology (e.g. contaminant spreading). We introduce a computationally efficient and numerically accurate method to estimate the one-point probability density (PDF) and cumulative distribution functions (CDF) of the wetting phase saturation for the stochastic Buckley-Leverett problem when the probability distributions of the permeability and porosity fields are available. The method is robust to high input variances and small correlation lengths, as well as complex geophysical profiles (e.g. anisotropy, channels). Once the saturation distribution is determined, any one-point statistics thereof can be obtained, especially the saturation average and standard deviation. Moreover, rarely available in other approaches, yet crucial, the probability of rare events and saturation quantiles (e.g. P10, P50 and P90) can be derived from the method. We validate the method with comparisons against Monte Carlo simulations.

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Taming parameter unidentifiability of ill-posed inverse problems in porous media

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ABSTRACT

Parameter unidentifiability is a significant problem for subsurface transport problems. For field-scale problems, spatially heterogeneous permeability values cannot be uniquely identified from measurements. This renders transport of solutes on the field-scale fundamentally uncertain. Methods for identifying these parameters such as traditional inverse analysis effectively ignore this uncertainty, but are computationally tractable. It is possible to find points of high-likelihood in parameter space that exhibit diverse transport behavior with Markov chain Monte Carlo (MCMC) methods, but often this comes with an exorbitant computational cost. We utilize a recently developed method that exists somewhere between these two methods to study uncertainty in the transport of solutes. Like MCMC, it is capable of finding points of high-likelihood in parameter space that exhibit diverse transport behavior, but it requires significantly less computational resources than a robust adaptive Metropolis MCMC method.

Identifying, estimating and quantifying uncertainty in hydrological modeling

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ABSTRACT

A hydrological model is a version of the reality or a model of it with errors. Typical sources of error include observation errors, initial/boundary conditions lack of control, unknown heterogeneity in parameters, scale discrepancy, model or system errors, and wrong choices on the mathematical representation of physico-chemical processes as well as in their numerical approximation. While modeling will always be subjected to uncertainty, an improved understanding of the sources of uncertainty and the ability to quantify the uncertainty could contributes significantly to improved management/decision-making practices.

The traditional approach of modeling and simulation dictates that one is usually aware of this ensemble of errors. They are taken into account, often in a primitive way, during calibration of models. During this phase of the modelling process one tries to find the parameter values of the model (e.g., hydraulic conductivity) such that the magnitude of the residuals is minimized. Once the model is calibrated, the errors are not explicitly taken into account for further predictions. With a stochastic approach, one tries to quantify the errors in model predictions. In practice, the exact values of the errors are not known in the model predictions. However, there is often some knowledge on the probability distribution of the errors from field observations. The probability distribution indicates the likelihood of an error pertaining to a certain value.

A set of examples are considered to evaluate the validity of the stochastic results through comparisons with Monte-Carlo simulations and field observations. The stochastic conductivity field generations using the Karhunen-Loeve expansion and the Turning Band method are compared against a resulting calibrated model, all honoring the field data/observations. The Distance Kernel method is used to identify clusters/redundancy in the field generations. The reduced set of conductivity realizations are then used in the simulation of flow and transport. The stochastic results are compared against the results obtained using the calibrated model approach. Examples demonstrate the reliability of numerical stochastic simulations and how the stochastic results can be used to estimate large-scale parameters. They further emphasize the limitations and extensions of the stochastic approach.

Error Quantification in Multiscale Methods

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ABSTRACT

Flow and transport in the subsurface can be described over a hierarchy of scales ranging from pore to continuum. Depending on the physical characteristics of the problem one may have to incorporate all relevant scales in any given computational model. This has led to the development of multiscale methods where a multiplicity of scales is modeled in the same simulation. One open challenge of multiscale simulations is to guarantee model predictivity once the coupling across scales is performed. In this work, we propose a general, robust and non-overlapping fully-coupled multiscale scheme based on Immersed Boundary Method (IBM) to model flow and reactive transport in porous media, where pore- and Darcy-scale equations are coupled together. The coupling conditions, obtained through a volume-averaging approach, allow one to preserve model predictivity once the coupling is performed, i.e. multiscale modeling errors can be bounded by the upscaling error of the coarser model deployed in the multiscale algorithm. The suggested algorithm is numerically tested for several transport and flow scenarios.

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Probabilistic Quantification of Environmental Performance Metrics for Risk Assessment

Presenter: Felipe de Barros
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ABSTRACT

Uncertainty quantification is one of the key challenges in contaminated groundwater driven risk analysis. For example, many of the factors that constitute human health risk assessment are uncertain and requires knowledge from multiple fields ranging from hydrogeology to public health. Improved understanding of the impact from each of these factors in risk estimation can provide guidance for decision makers to better manage contaminated sites and allocate resources towards characterization efforts. In this presentation, I will focus on the impact of aquifer heterogeneity in environmental performance metrics, e.g. human health risk measures and solute concentration. Spatial heterogeneity of the hydrogeological properties can lead to the formation of preferential flow channels which control the contaminant plume spreading rates and travel time statistics, both which are critical in assessing the risk level. Through the use of an integrated hydrogeological-health stochastic risk framework, the significance of characteristic length scales (e.g. characterizing flow, transport and sampling devices) and aquifer heterogeneity in controlling the uncertainty of environmental performance metrics is highlighted.

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An efficient algorithm for estimating the least resistance path in spatially heterogeneous porous media

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ABSTRACT

The dynamics of a solute plume migrating through a heterogeneous porous formation are strictly related to the physical hydrogeological properties and external forcing factors (e.g. boundary conditions, sinks and sources). Many studies have shown that the heterogeneity of the hydraulic conductivity field is one of the main factors for understanding and predicting the solute transport phenomena in the subsurface. For example, higher levels of subsurface heterogeneity enhance the probability of having high connectivity paths which will have an impact on overall solute plume transport behavior. Such preferential paths are fundamental in predicting the first time arrivals and in tracking the plume advancing front, both which are critical for risk analysis [1]. In this work, we establish a statistical link between static measures related to the hydraulic conductivity field with relevant dynamic quantities such as solute travel times and other environmental performance metrics within a probabilistic framework. Although some analytical results have been obtained in the past they were limited to low heterogeneity [2] and the issue related to transport in highly connected formations is still subject of current research efforts. Here, the static quantities taken into consideration are the hydraulic resistance and the corresponding least resistance paths [3]. In this work, we present an efficient novel algorithm for extracting information solely based on the hydraulic conductivity field and can be used to estimate the connectivity of subsurface environment. Due to its efficiency, an exhaustive and fast computational analysis can be carried out using a high resolution Monte Carlo approach in the context of probabilistic risk assessment.

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On the role of uncertainty quantification in pore-scale physics

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ABSTRACT

Uncertainty quantification (UQ) techniques are commonly used at the field scale for coping with limited knowledge of porous media parameters, both to assimilate data and to provide predictions with an estimation of the associated uncertainty. However similar problems seem to be underestimated when dealing with problems at the lab or pore-scale. This can be explained by the complexity of the physical models and numerical simulations. Nevertheless, issues like model validation, calibration, parametric uncertainty, spatial variability of pore samples, can be conveniently addressed by UQ techniques. We highlight the role that UQ can play in pore-scale problems, with two examples: namely a forward propagation of uncertainty in pore-scale simulations of flow and transport by means of multilevel Monte Carlo, and a Bayesian validation study as an alternative to deterministic upscaling methods for multiphase flows.

Uncertainty analysis of the chemical injection in enhanced oil recovery (EOR)

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ABSTRACT

The presence of large uncertainties due to limited/noisy experimental data is a major challenge in numerical reservoir simulations. These uncertainties are expressed in terms of probability distributions on the model inputs and are interpreted as degrees of belief about the true, albeit unobserved, values of these parameters. In consequence, individual deterministic reservoir simulations are not reliable. Truly predictive simulations must take into account input uncertainties and be able to provide rigorous error bars for the model outputs. Uncertainty analysis becomes further important for costly and complicated EOR techniques such as chemical flooding where numerous uncertainties are involved. In this work, we study the effect of such uncertainties on a chemical flooding EOR field project. In particular, we consider uncertainties in reservoir porosity, relative permeability, and polymer's and surfactant's absorption isotherms. The latter two are model-form uncertainties induced by the lack of adequate field measurements and have not been studied elsewhere. Our work consists of two stages. First, we construct stochastic models for all uncertain quantities by combining our physical knowledge with experimental measurements. This endeavor involves a combination of random field theory and Bayesian statistics. Second, we propagate these uncertainties through the reservoir model using state-of-the-art high-performance computational methods. We show how our findings can be used to gain insights into which experiments we should do in order to reduce predictive uncertainty. The reservoir model is implemented using the MATLAB reservoir simulation toolbox.

Characterization of rock properties in a poroelastic medium with Markov chain Monte Carlo method

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ABSTRACT

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 [Murad et al., 2013]. The coupling of geomechanical effects and fluid flows is widely influenced by the rock heterogeneity [Frías et al., 2004, Abbasi et al., 2007, Mendes et al., 2012] 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. In this sense, inverse problems are used to infer about the model parameters on the basis of observation (dynamic) data and to obtain a more reliable prediction of the processes. More specifically, here we use the Markov chain Monte Carlo Method to characterize the porosity, permeability and Young's Modulus using pressure, production and subsidence data for a slightly compressible two-phase flow in a poroelastic medium.

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Some new approaches to simulating two-phase flow in porous media on hexahedral meshes

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ABSTRACT

Subsurface geology often dictates that relatively general hexahedral computational meshes be used when simulating flow in porous media. The equations of two-phase flow divides into a parabolic pressure equation for the flow and a degenerate parabolic (convection-diffusion) saturation equation for the transport. We present three new approaches. (1) The elliptic part of both equations is often approximated using mixed finite elements, which are defined by mapping from a reference cube using the Piola transformation. This destroys the approximation properties of the method. We describe a new family of finite elements (AC elements) that overcomes the problem. (2) The saturation equation exhibits degeneracy in its elliptic diffusion term due to loss of capillarity when a phase is lost. We present a new mixed formulation that is stable when approximating degeneracies. It is suitable for approximation with the new AC elements. (3) The convection part of the saturation equation is often approximated, for example, using discontinuous Galerkin (DG) methods, since DG can handle general meshes. Traditional WENO methods are very accurate but restricted to rectangular meshes. We present a new approach using high order WENO reconstructions on logically rectangular meshes.

New preconditioning strategy for Jacobian-Free solvers for variably saturated flows with Richards' equation

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ABSTRACT

In a wide variety of environmental applications variably saturated flow in porous media is a critical process which is often modeled by Richards' equation. In Richard's formulation the flow model is considered under the assumption that the gas phase is immobile. This simplification also makes Richards' equation a strongly nonlinear parabolic PDE, creating significant challenges for the performance of nonlinear solvers.

The implicit discretization in time of its mixed-form is the standard approach for this type of applications since it enables large time steps and locally conserve mass. This scheme leads to a nonlinear discrete system of equations that must be solved at each time step. The geometric complexity of the subsurface environment requires to handle non-orthogonal and unstructured meshes. To discretize the flow model in these settings advanced discretization methods are essential. These methods offer accurate schemes on general meshes, but close-from formulas for the analytic Jacobian may not exist, e.g slope-limiting methods, nonlinear discretization schemes. For these discrete systems an implementation of the standard Newton-Raphson-type nonlinear solvers becomes very problematic. Therefore, development of Jacobian-Free solvers has attracted a lot of interest in the past decade.

Several Jacobian-Free methods have become quite popular in the recent years. Methods, such as the Jacobian-Free Newton-Krylov method, only require the action of the Jacobian matrix on a vector, which is approximated via the numerical computation of the Gateaux derivative. Accelerated fixed-point methods such as Anderson Mixing and Nonlinear Krylov Acceleration (NKA) methods are design to extend the power of linear iterative schemes to the nonlinear case. In all of these methods the preconditioner plays a crucial role for the efficacy of a nonlinear solver. The standard preconditioning approach is based on a linearized counterpart of the original discrete system. The strong nonlinearity in the coefficients limits the efficacy of that approach and results in the growth of nonlinear iterations.

We propose and analyze a new preconditioning strategy that is based on a stable discretization of the continuum Jacobian. The underlying idea in this work is to reverse the order of the discretization and linearization steps in the development of the nonlinear solver. Specifically, by performing the linearization step first, the analytic Jacobian of the continuum model is derived and then analyzed to establish requirements for accurate and stable discretizations. This strategy allows us to take full advantage of advanced discretization methods. For example, we may use monotone schemes for the diffusive term in the Jacobian and upwinded schemes for the advective term. This not only leads to an efficient preconditioner but also allows us to control its numerical properties. The proposed strategy was tested in simulations of water infiltration into a partially saturated layered medium in steady-state and transient regimes on non-orthogonal subsurface topology with heterogeneous permeabilities and water retention models. These experiments demonstrate that the new preconditioner improves convergence of the existing Jacobian-Free solvers 3-20 times.

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Coupled multipoint flux and multipoint stress mixed finite element methods for poroelasticity

Presenter: Ivan Yotov
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ABSTRACT

We discuss mixed finite element approximations for the Biot system of poroelasticity. We employ a weak symmetry elasticity formulation with three fields - stress, displacement, and rotation. We study two elasticity formulations, with poroelastic and elastic stress as primary unknown, respectively. Stability bounds and error estimates are derived for both formulations for arbitrary order mixed spaces. We further develop a method that can be reduced to a cell-centered scheme for the displacement and the pressure, using the multipoint flux mixed finite element method for flow and the recently developed multipoint stress mixed finite element method for elasticity. The methods utilize the Brezzi-Douglas-Marini spaces for velocity and stress and a trapezoidal-type quadrature rule for integrals involving velocity, stress, and rotation, which allows for local flux, stress, and rotation elimination. We perform stability and error analysis and present numerical experiments illustrating the convergence of the method and its performance for modeling flows in deformable reservoirs.

Nonconforming three field discretization of Biot's model in poroelasticity

Presenter: Xiaozhe Hu
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ABSTRACT

A stable and oscillations free finite element scheme for a three-field Biot’s model in poroelasticity is considered. The involved variables are the displacement, Darcy velocity and the pore pressure, and they are discretized using the lowest approximation order: Crouzeix- Raviart finite elements for the displacements, lowest order Raviart-Thomas elements for the fluid flux, and piecewise constant approximation for the pressure. We show convergence of the discrete scheme which is implicit in time and use these types of elements in space. Finally, numerical experiments illustrate the convergence of the method and show its effectiveness to avoid spurious pressure oscillations.

Generalized Multiscale Finite Element Method for Simulations of Flows in Porous Media

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ABSTRACT

In this talk, I will describe a general local multiscale model reduction technique for simulations of porous media processes. The method is designed to solve multiscale problems on a coarse grid, where the coarse-grid size is much larger than the smallest spatial scale for heterogeneities. The method starts with local snapshots and local spectral problems. I will describe some of main ingredients of the method and applications to various problems. I will discuss the relation to numerical upscaling and it can be combined with upscaling methods.

Monotone nonlinear finite-volume method for nonisothermal two-phase two-component flow in porous media

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ABSTRACT

Flow and transport phenomena in porous media are the governing processes in many geological, industrial and biological systems. These processes occur on different spatial and temporal scales. It is therefore important to develop numerical schemes which are efficient and robust enough to handle usually highly anisotropic heterogeneous large-scale problems. Applications differ from energy storage in the subsurface to nuclear waste storage up to drug transport through human tissue. Modeling such processes results in highly nonlinear partial differential equations, that often have to be solved on unstructured and non-conforming grids, to fulfill geometric constraints. Due to the additional requirement of mass-conservation, the most commonly used methods for solving flow problems in porous media are Multi-Point Flux Approximation methods, Mixed Finite Element methods, or Mimetic Finite Difference methods.
In terms of accuracy, these schemes converge at least with second order for the considered variable and first order for the fluxes. That means, they are exact for linear and piecewise linear solutions. The major drawback of these schemes is the fact that they are not unconditionally monotone, which means that maximum and minimum principles are not satisfied for arbitrary grids and permeability tensors. Non-monotone schemes may produce unphysical solutions, which in turn influence the efficiency and convergence of the scheme. It is proven that there exist no linear higher order unconditionally monotone control volume schemes.

Relaxation of this linearity requirement allows the construction of monotone schemes. The first idea of a nonlinear scheme that is monotone on triangular grids has been published by Le Potier [1]. Recently, this scheme has been
extended to polygonal meshes [2]. Most of the existing literature about nonlinear finite-volume schemes focuses on linear elliptic equations. Only a few publications exist that consider multi-phase flow in porous media [3].
However, they do not account for compositional and nonisothermal effects.

We will present a numerical analysis of accuracy and efficiency of a nonlinear finite-volume scheme for the nonisothermal two-phase two-component porous media flow equations. Furthermore, the influence of nonlinear schemes on the numerical behavior will be shown in detail. We demonstrate that these nonlinear flux approximations may positively influence the convergence behavior of nonlinear and linear solvers, due to the fact that condition numbers of occurring Jacobian matrices are reduced compared to linear methods. Finally, we will exhibit that these schemes can solve benchmark problems as accurate as linear methods.

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Modeling of enhanced oil recovery on general hexahedral grids

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ABSTRACT

Accurate numerical simulations are required for design and evaluation of enhanced oil recovery strategies such as ASP (Alkaline Surfactant Polymer), foam and low salinity flooding. We discuss the significance of accurate fluxes for non-Newtonian viscosity calculations. Multipoint Flux Mixed Finite Element (MFMFE) method [1] is used for discretization. This improves concentration and saturation front predictions owing to better calculation of advection, diffusion and dispersion terms. The numerical results show the effect of accurate fluxes on recovery predictions.

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Implementing Multipoint Flux Mixed Finite Elements on Non-Matching Hexahedral Grids Using the Local Flux Method

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ABSTRACT

In this work we develop an extension of the Multipoint Flux Mixed Finite Element (MFMFE) method [1] to allow discretizations on non-matching distorted hexahedral multiblock grids. This is accomplished by employing techniques from the Local Flux (LF) Mimetic Finite Difference Method [2], in which the velocity space is enriched on subdomain interfaces and elements adjacent to subdomain interfaces are treated as general polyhedra with extra faces in a mimetic fashion. Special quadrature rules are used to reduce the saddle point system to a positive definite system in the pressure variable. Our method is demonstrated to be an efficient way of performing local grid refinement in a mixed method without the overhead of fully unstructured grids. It is also shown to be accurate and we obtain optimal convergence rates in appropriate norms.

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A Lagrange multiplier method for flow in fractured poroelastic media

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ABSTRACT

We study the finite element computational model for solving coupled
problem arising in the interaction between a poroelastic material and a fracture
filled with fluid. The fluid flow in fracture is governed by the Stokes equation
for an incompressible fluid, while the poroelastic material is modeled using the Biot
system. The appropriate equilibrium and kinematic conditions are imposed on the interface. The focus is made on the approximation of the interface conditions, which feature the interaction of different variables. The Lagrange multiplier method is used
to enforce these non standard interface conditions. After performing the stability and error analysis, a series of numerical experiments were done in order to study the convergence rates, the applicability of the method to modeling physical phenomena and sensitivity of the model with respect to its parameters.

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A multipoint stress mixed finite element method for elasticity

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ABSTRACT

We develop a new mixed finite element method for linear elasticity model with weakly enforced symmetry on both simplicial and quadrilateral grids. Motivated by the multipoint flux mixed finite element method for flow in porous media, we consider a special quadrature rule that allows for elimination of stress and rotation variables and leads to a cell-centered system for the displacements. Theoretical results indicate the stability of method and predict first-order convergence for all variables in the natural norms, numerical experiments confirm the theory for both types of meshes.

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A linearization scheme for two phase flow in a porous medium

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ABSTRACT

We discuss a new linearization scheme for two phase flow in a porous medium. The model consists of a degenerate parabolic elliptic saturation equation coupled to an elliptic pressure. Our scheme is based on using the global pressure formulation and using the Kirkchoff transform to obtain the saturation equation with a linear diffusion term. The scheme is a linear and iterative and consists of solving the pressure equation followed by the saturation update. The scheme consists of lagging the time derivative saturation term and using a linearization of the time derivative term.
We analyse the scheme and show the convergence of the scheme to the continuous equation. In addition, we derive the error estimates for the numerical approximations. We extend the work for the Ho ?lder continuous functions.

Convergence of iterative schemes for coupled flow and geomechanics in a fractured reservoir

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ABSTRACT

Coupling of geomechanics and flow in a poroelastic porous media has several applications including subsidence events, ground water remediation, hydrocarbon production, enhanced geothermal systems, solid waste disposal, hydraulic fracturing, biomedical modeling and geological carbon sequestration. The fact that the fractures in the porous media have strong influence on the flow profiles and the defor- mations are particularly significant in such reservoirs motivates studying the coupled geomechanics and flow problems in fractured reservoirs.
We report here some of the developments in suitable iterative schemes and their analysis for fractured porous media. Our work has two components: 1. Development of iterative scheme by decoupling the flow and mechanics solve, 2. Developing multirate schemes by exploiting the different time scales of mechanics and flow solve by taking coarser time step for mechanics and smaller time steps for flow. The iterative multirate schemes combine the advantages of both implicit and explicit approaches. They are efficient, allow larger time steps, are robust, and the decoupling allows us to solve the linear systems efficiently.

One-Way Model for Three-Phase Flow In Highly Heterogeneous Poroelastic Media

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ABSTRACT

In this work we present a conservative numerical methodology for solving three phase compressible flow in strongly 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 evolving algorithm is constructed based on implicit discretization of the hydrodynamics and explicit for the saturations. The nonlinearities inherent to the coupling between pressure and saturation equations are handled by a proper sequential iterative scheme. Furthermore, the system of conservations laws is rephrased in an alternative form with an extra source term arising from the transient Lagrangian porosity induced by the geomechanical coupling. 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]. A reduced version of the new iteratively coupled method, based on the one way formulation applied to incompressible liquid phases and a fully compressible gas phase, is discretized by sequential locally conservative numerical schemes. Numerical simulations of problems in poroelastic media are performed showing the potential of the methodology proposed herein

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A 3D coupled HM-XFEM model for fluid driven fractures in porous media

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ABSTRACT

Rock permeability is strongly influenced by the presence of fractures, which represent a prevailing path for the fluid flow. In some cases such fractures are an important factor for reservoir productivity and often, in the case of low permeability rocks, methods to increase permeability, like hydraulic fracturing, are used in order to make the reservoir economically exploitable. On the contrary, in other cases the presence of fractures is detrimental, as in CO2 storage, for which the gas flow through the fractures in the reservoir seal and faults reactivation represent a major concern. It is therefore important to be able to predict the effect of the presence of such fractures in a reservoir: pressure response, recovery, impact of subsidence or heave during production. The aim of this work is the development of a numerical technique for the simulation of hydraulic fracture propagation.
In the following, we introduce a new finite element to model the coupled effects of groundwater flow and fracture evolution in a fractured porous medium submitted to local or regional stress-state variations. An enriched finite element formulation is preferred to a standard formulation in order to overcome the difficulties brought by the presence of arbitrary discontinuities. The internal interfaces are then taken into account by additional degrees-of-freedom so that the finite element mesh does not need to conform to the fracture geometry.

The discontinuous shape functions associated to these additional degrees-of-freedom simulate the presence of fractures in the medium. Therefore the XFEM method [1], based on the partition of unity [2], is employed to discretize the variational formulation of the fully-coupled Hydro-Mechanical (HM) problem.
The partially saturated porous-mechanical model developed by Khoei & al. [3] provided us a basis for the establishment of our model. It includes both discontinuous displacement and pore pressure fields across the fracture. We complete this work with the introduction of two additional fields:
the fluid pressure field generated by the flow through and inside the fracture,
a Lagrange multiplier field resulting from the dualisation of the pressure continuity condition (at the fracture wall) between the pore pressure and the fluid pressure inside the fracture allowing us to model permeable fractures as well as non-permeable fractures.
Under the assumption of small perturbations, the fracture aperture is driven by the fluid flow which itself depends on fracture aperture due to the Cubic law. A non-regularized cohesive law is adopted to handle the fracture evolution [4], allowing us to propagate the fractures along non predefined paths.
The model is implemented in EDF's software Code_Aster. In order to ensure numerical stability of the model, cautions must be taken. In particular the numerical LBB condition has to be satisfied. To fulfill this requirement close to the fracture:
quadratic shape functions are used to for the interpolation of the displacement field close to the fracture and linear shape functions for the pore pressure, the fluid pressure and the Lagrange multiplier

Modeling Gas Migration in Poro-Fractured Media due to Barometric Pumping

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ABSTRACT

Poro-fractured media subjected to barometric pressure variations results in enhanced gas migration compared to a single-continuum media. Barometric pressure variations access deeper portions of the media via fractures, resulting in the “barometric pumping” effect. For example, considering reasonable hydraulic properties, fractures can be expected to carry 99.999% of vertical mass flow (Nilson et al, 1991). Gas migration is further enhanced by gas solubility in relatively immobile fluids present in the pore spaces of the media (i.e., liquid-filled pore space in the matrix material). Gas solubility provides a “ratcheting mechanism”, whereby gas migration is not completely reversed due to high-pressure events. Each high-pressure event leaves behind dissolved gas that exsolves during the subsequent low-pressure event to be transported further from the source. Modeling the physical processes controlling gas migration in poro-fractured media subjected to barometric pumping is crucial for understanding radionuclide gas breakthrough at the ground surface from an underground nuclear test, passive vapor extraction of contaminated ground, and landfill gas migration.
We will describe an application of modeling gas migration in poro-fractured media subjected to barometric pumping. The application is based on migration of Xe-133 from an underground nuclear test. Damage models are generated by the CASH hydrodynamic rock damage code based on explosions at various depths for given rock properties. Meshes are generated based on the damage models using the Los Alamos Grid Toolbox (LaGriT; http://lagrit.lanl.gov), where areas with greater damage are refined to greater detail. We model gas migration using a generalized-dual-permeability model (GDKM) within the Finite Element Heat and Mass transfer (FEHM; https://fehm.lanl.gov) code. We estimate representative, heterogeneous fracture permeabilities based on the cubic law (kf=?f2/12, where ?f is the fracture aperture derived from the damage model). Comparisons of simulated pressures and gas migration to existing analytical solutions will be presented. Use of the simulations to forecast travel time and surface concentrations of Xe-133 will be discussed.

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Simulation of the flow in complex networks of fractures with a robust optimization approach

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ABSTRACT

The effective simulation of the flow in the underground is a challenging task, of great importance for many practical applications, such as the enhanced production of oil and gas, the geological disposal of pollutants or of nuclear waste, water resources management or geothermal applications. Among others, 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. Such networks are stochastically generated starting from probability distributions of 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 lengths, 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.
A new simulation approach has been recently proposed in order to efficiently solve the steady state flow in DFNs, overcoming the above mentioned difficulties. The method is based on a PDE-constrained optimization formulation, on non-conforming meshes and uses unconventional discretization techniques, such as the XFEM or the VEM, to represent the solution. The idea at the basis of the new approach consists in splitting the original problem into many fracture-local sub-problems, resorting to the minimization of a cost functional to enforce matching conditions at the interfaces of the sub-problems. The same functional is also used to impose boundary conditions, in order to limit the geometrical handling of the complex and large computational domains of realistic DFNs. The method has a strong parallel nature, allowing for the simulation of large networks. A strategy to solve heterogeneous networks with the optimization approach is also described.
Numerical simulations are proposed on large networks with complex geometries and heterogeneous hydraulic properties. Error indicators have been identified in order to provide estimates for the quality of the obtained solution, also allowing for a comparison of the solution on networks with very different characteristics. The obtained numerical results have shown the effectiveness of the method in tackling complex and large networks, highlighting the robustness of the approach in handling the complexities related to the simulation of the flow in realistic DFNs.

Stefano Berrone, Sandra Pieraccini, and Stefano Scialò. A PDE-constrained optimization formulation

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Space-time domain decomposition method for two-phase flow model in a porous medium

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ABSTRACT

We consider a simplified model for a two-phase flow model through a heterogeneous porous medium. The porous medium is made up of different sub-domains, each of them being a different rock type. Each rock is characterized by its relative permeability and capillary curves that are functions of the phase saturations. Domain decomposition provide a natural approach for dealing with the different physics occurring in the different rock types, which induces a discontinuity of the saturation (see Fig 1).

We propose a global in time domain decomposition, which gives us the flexibility to use different time steps. More precisely, focusing on the capillary forces motion, we propose a new approach based on optimized Schwarz waveform relaxation (OSWR), with nonlinear Robin conditions in the context of nonlinear degenerate parabolic problem. We propose and analyze a hybridized finite volume scheme for the approximation of the multi-domain solution. The well-posedness of the local subdomain problem with Robin boundary condition is proved by the convergence of the discrete solution. The well-posedness of the discrete coupled multidomain solution is then derived. To accelerate the convergence of the OSWR method, we reformulate the multidomain problem as a nonlinear interface problem whose unknowns are Robin data on each side of the interface, and for which more general non-linear solvers can be used (Newton-like solvers). Such an interface problem is global in time, thus different time grids are employed to adapt to different time scales in the different rock types. In particular, such approach can be useful when the physical domain contains fractures or barriers between different rock types (by using different time scales in the subdomain and in the fractures/barriers). The choice of Robin parameters will be studied, as well as its influence on the global domain decomposition method. Numerical results for three-dimensional problems for domains with different
capillarities are presented to illustrate the performance of the method. More realistic prototypes for simulations for the underground storage of nuclear waste
are shown.

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dfnWorks: An HPC Workflow for Discrete Fracture Network Modeling with Subsurface Flow and Transport Applications

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ABSTRACT

A workflow, dfnWorks, generates discrete fracture networks (DFN) of planar polygons, creates a high quality conforming Delaunay triangulation of the intersecting DFN polygons, assigns properties (aperture, permeability) using geostatistics, sets boundary and initial conditions, solves pressure/flow in single or multi-phase fluids (water, air, CO2) using the parallel PFLOTRAN or serial FEHM, and solves for transport using Lagrangian particle tracking. We outline the dfnWorks workflow and present applications from a range of fractured rock systems.

dfnWorks (http://www.lanl.gov/expertise/teams/view/dfnworks) is composed of three main components, all of which are freely available. dfnGen generates a distribution of fracture polygons from site characterization data (statistics or deterministic fractures) and utilizes the FRAM (Feature Rejection Algorithm for Meshing) to guarantee the mesh generation package LaGriT (lagrit.lanl.gov) will generate a high quality conforming Delaunay triangular mesh. dfnWorks links the mesh to either PFLOTRAN (pflotran.org) or FEHM (fehm.lanl.gov) for solving flow and transport. The various physics options available in FEHM and PFLOTRAN such as single and multi-phase flow, water, CO2 and reactive transport are all available with appropriate initial and boundary conditions and material property models. dfnTrans utilizes explicit Lagrangian particle tracking on the DFN using a velocity field reconstructed from the steady state pressure/flow field solution obtained in PFLOTRAN or FEHM.

Applications are shown for a nuclear waste repository in fractured granite, CO2 sequestration and the multi-phase displacement of water by CO2 in fractured rock and hydraulic fracturing and extraction of unconventional hydrocarbon resources.

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An Integrated Geological and Mathematical Framework for Geothermal Reservoirs

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ABSTRACT

Enhanced geothermal systems (EGS) in reservoirs are based on circulation of fluids, mainly water, in fracture networks. Fractures are planar or sub-planar discontinuities along which a rock has been broken, and represent important conduits for fluid flow. This is of particular importance for geothermal reservoirs, as matrix porosity and permeability is generally on a negligible scale. Furthermore, fractures increase the contact surface between rocks and fluids, facilitating a crucial contribution to heat transport by conductive heat exchange between fluids and the surrounding rock mass. Despite a global wealth of knowledge of fractured reservoirs, it is unclear which set of fracture parameters (type, level of detail, scale, accuracy) that provide the most direct route to realistically predicting flow properties. Geological modeling and simulation are hence both crucial ingredients for assessing the commercial viability of production strategies for fractured geothermal reservoirs. Our presentation is focused on a mathematical and geological framework which combines traditional geometric fracture data with topological information, under the hypothesis that the latter may contribute more information on percolation properties of the network [SN15]. Simulations with real fracture geometries, as well as synthetic but based on the previous considerations, are performed in a three-dimensional discrete fracture network (DFN) setting, see [FFSR14, BBPS14], which can be viewed as a screening tool in data processing. The numerical method consider the fractures as objects of co-dimension one and include the aperture in their mathematical description moreover is able to handle non-conforming fractures intersections giving a high freedom in the simulations. The long term vision of our work is to develop an integrated geological and mathematical framework for collection and mutual transfer of data between geological and simulation models for EGS.

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Numerical simulation of fault and fracture mechanics

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ABSTRACT

The simulation of the mechanics of geological faults and fractures is of paramount importance in several applications, such as ensuring the safety of the underground storage of wastes and hydrocarbons or predicting the possible seismicity triggered by the production and injection of subsurface fluids. However, the stable numerical modeling of ground ruptures is still an open issue. The present work introduces a novel formulation based on the use of the Lagrange multipliers to prescribe the constraints on the contact surfaces. The variational formulation is modified in order to take into account the frictional work along the activated fault portion according to the principle of maximum plastic dissipation. The numerical model is developed in the framework of the Finite Element method and gives rise to a discrete non-linear system of equations whose Jacobian matrix has a non-symmetric generalized saddle-point structure. The proposed formulation proves able to provide stable solutions with a fast convergence of the non-linear problem. The computational efficiency can be further improved by using an appropriate preconditioned Krylov subspace method for the solution of the inner linearized steps.
The numerical model of faults and fractures is tested in a set of numerical examples against analytical solutions. Finally, two realistic applications are investigated, dealing with the generation of ground fractures due to groundwater withdrawal in arid regions and the possible seismicity triggered by underground gas storage in a faulted hydrocarbon reservoir.

Upscaling two phase flow within naturally fractured reservoirs : a new and original approach to characterize block size and to upscale parameters

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ABSTRACT

Modeling and Upscaling two phase flow within naturally fractured reservoirs (NFR) is a challenging area of study within the global fractured reservoir simulation issue. In fact, fine grid simulation involving grid cell size down to millimeters rises both numerical, computational and memory issues (Fourno, and al., 2011), (Noetinger and Jarrige., 2011). In order to avoid explicit fine grid simulations, dual medium formulation is used (Barenblatt, and al., 1960). This formulation considers both fracture and matrix media separately with a flux occurring between the two media thanks to an exchange equation. There are two dual medium models. The first model is the dual porosity single permeability : large scale flow occurs exclusively in fracture medium, the matrix acting as a reservoir by means of an exchange term. The second model is the dual porosity dual permeability: large scale flow occurs in both fracture and matrix media simultaneously, in addition to the exchange term. These models can provide accurate results if the equivalent parameters in both media are correctly evaluated (equivalent permeability, relative permeability curves, equivalent matrix block size, etc…). This process of computing equivalent parameters knowing the microstructure of the medium is called upscaling. The upscaling method depends on the physical phenomena controlling the matrix-fracture exchanges (gravity, capillarity and viscosity) (Lemonnier et al., 2010).

A new and original approach to derive equivalent matrix block size is presented. This approach is based on the main flow directions of the Discrete Fracture Network (DFN). The main contribution of this method is that the derived representative matrix block is oriented following the main flow directions. In addition, this approach is also three dimensional and has a very low computational time. Considering this new block size approach and with the hypothesis that flow and matrix-fracture exchanges are exclusively controlled by viscous effects, a two phase flow upscaling workflow is presented. The main steps of this workflow are: upscaling fracture medium, deriving the representative matrix block and upscaling matrix medium.

The new equivalent block size derivation approach is applied to a NFR grid cell scale. The NFR model contains two randomly generated fracture families. Two validation cases are considered. In a first test, the mean spacing of both fracture families is varied. In a second test, the relative orientation between the two fracture families is varied. The new method gives expected results knowing fracture spacings and fracture orientations and presents also the outcome of being faster compared other classical methods.

The upscaling workflow is applied to a 2D vertical NFR section of a reservoir cell grid scale. Gravity and capillarity effects are neglected and only viscous forces are considered. Different situations of the matrix medium are considered (homogeneous or heterogeneous in term of permeability, porosity and relative permeability curves). A dual model is obtained using the proposed workflow. This dual medium model is validated against fine grid reference simulations. In term of recovery curves, a good agreement is obtained with acceptable computational cost.

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The Virtual Element Method for Discrete Fracture Network flow simulations

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ABSTRACT

The simulation of subsurface fluid flows has applications in a wide range of fields, including e.g. oil/gas recovery, gas storage, pollutant percolation, water resources monitoring, CO2 geological storage, geothermal applications, nuclear waste disposal. Underground fluid flow in fractured media is a heterogeneous multi-scale phenomenon that involves complex geological configurations; a possible approach for modeling the phenomenon is given by Discrete Fracture Networks (DFNs), which are complex sets of polygonal intersecting fractures generated starting from random distributions for geometrical features (such as orientation in the three dimensional space, position, dimension, and aspect ratio) and hydrogeological properties (trasmissivity). Geological fractured media are therefore characterized by a very challenging geometrical complexity, which is one of the major difficulties to be tackled when performing DFN flow simulations.
This talk concerns the application of the Virtual Element Method [1] to the steady state simulation of the flow in DFNs [3, 5, 6]. In this approach we can exploit the flexibility of VEM in order to tackle the geometrical complexity. Indeed, a crucial issue in DFN flow simulations is the need to provide on each fracture a good quality mesh on any randomly generated configuration. Namely, if classical triangular or quadrilateral meshes on the fractures are required to be conforming to the traces (fracture intersections), and also conforming each other, the meshing process for each fracture is not independent of the others, thus yielding in practice a quite demanding computational effort for the mesh generation process. In some cases, the meshing process may even result infeasible so that some authors propose to modify the DFN removing problematic fractures.
Here, the VEM will be used within several possible approaches to the problem: in conjunction with a newly conceived PDE-constrained optimization approach [2, 3, 4], in conjunction with a mortar approach [5] introducing a partially conforming mesh, as well as on a totally conforming polygonal mesh [6].
Indeed, taking advantage from the great flexibility of VEM in allowing the use of rather general polygonal mesh elements, a suitable mesh for representing the solution and imposing matching conditions between the solutions on different fractures can be easily obtained, starting from an arbitrary triangular mesh independently built on each fracture, and independent of the trace disposition. An optional mesh smoothing step can improve the quality of the polygonal mesh. Robustness and efficiency of the approach allow the application of the method to quite large and complex DFNs involving very complex geometrical situations like, for example, very small angles (less than one degree), coexistence of large and small fractures and long and very short fracture intersections.

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An arbitrary-order accurate mimetic finite difference method for flows in porous media.

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ABSTRACT

We present an arbitrary-order accurate Mimetic Finite Difference (MFD) method for the approximation of time-dependent diffusion problems in mixed form on unstructured polygonal and polyhedral meshes.
The method requires the definition of a high-order approximation of the divergence and gradient operators and of two inner products for the discrete analogs of fluxes and scalar unknowns.
The discrete divergence and gradient operators are built according to a discrete duality relation.
The inner product for the flux grid functions is built by explicitly imposing the conditions of consistency and stability.
The family of semi-discrete mimetic methods is proved theoretically to be energy-stable as the corresponding continuous problem.
Then, a full discretization is derived by combining the MFD method of order k with time marching schemes from the Backward Differentiation Formula (BDF) of order k+2.
Numerical experiments confirm the accuracy by solving the
time-dependent diffusion problems with a variable diffusion tensor for k from 0 to 3 on three different mesh families.

Multiscale simulations of reactive transport in fractured media

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ABSTRACT

Darcy-scale models of flow and transport in porous and fractured media often fail to describe experimentally observed phenomena, while their pore-scale counterparts are accurate but can be computationally prohibitive. Most numerical multiscale models, which seek to combine these two descriptions, require empirical closures and/or assumptions about the behavior of pore-scale quantities at the continuum (Darcy) scale. We present a general formulation of an iterative hybrid numerical method that links the pore and continuum scales without resorting to such approximations. The algorithm treats the fluxes exchanged at the internal boundaries between pore- and continuum-scale domains as unknown, and allows for iteratively determined boundary conditions to be applied at the pore-scale in order to guarantee flux continuity. While the algorithm proposed is general, we use it to model transport in a fracture with chemically reactive walls. Results demonstrate significant improvement upon standard continuum-scale formulations.

An original and useful approach to mesh a discrete fracture network

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ABSTRACT

Modeling mass and heat transfers in fractured media is a challenge. That is due to the geometrical complexity of the discrete fracture network (DFN) and the remaining input data uncertainties. As an illustration, in the field of CO2 sequestration or oil reservoir production, transfers have to be modeled at the scale of reservoirs (¼ 10km¤10km) using ¼ 100m¤100m¤10m grid cell sizes, [1]. However, fractures are finely characterized on well logs and outcrops (at a scale of few meters). From this characterization a DFN can be built and may contain over 106 fractures. Analogous issues are to be adressed for hydrology and geothermal applications. Direct numerical simulations taking into account the DFN geometry remain still impossible at the reservoir scale. In practice, upscaling approaches are used to determine equivalent transfer parameters at the grid cell scale. The number of fractures belonging to a grid cell and respecting data from characterization scale may be close to 103 fractures. This number is more tractable and direct numerical simulation may be used at this step. Nevertheless, considering the complexity of the DFN geometry, it still remains to simplify the DFN mesh, considering assumptions about the details of the flow [2, 3, 4]. In order to test the accuracy of these assumptions, reference numerical simulations must be carriedout using a mesh which accounts for the detailed DFN geometry [5]. The goal of this paper is to present an original 3D DFN mesh approach allowing to get high fidelity reference simulations and allowing to test further simplifications required by applications.

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The nonconforming virtual element method

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ABSTRACT

In this poster, we present the unified framework for conforming and noncon- forming Virtual Element Method (VEM) for the numerical treatment of elliptic problems. This formulation works on very general unstructured meshes in 2D and 3D, and is the same for any polynomial order of accuracy. For advection- diffusion-reaction problems, the differential operator is split into its symmetric and non-symmetric parts and conditions for stability and accuracy on their dis- crete counterparts are established. Numerical experiments verify the theory and validate the performance of the proposed method.

Application of dfnWorks to Modeling ?Natural Gas Production, Studying the Effect of Injection Mode Boundary Conditions, Water Loss in Hydraulic Fracturing and The Effect of Internal Aperture Variability on Transport

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ABSTRACT

A workflow, dfnWorks (http://www.lanl.gov/expertise/teams/view/dfnworks), generates discrete fracture networks (DFN) optimized for modeling flow and transport in fractured rock systems. We present a series of four applications of the dfnWorks capability to modeling flow and transport in fractured rock systems.??

1) With realistic three-dimensional representations of fracture network geometry and aperture variability, simulated production decline curves qualitatively resemble observed production decline curves. The high initial peak of the production curve is controlled by advective fracture flow of free gas within the network and is sensitive to the fracture aperture variability. Matrix diffusion does not significantly affect the production decline curve in the first few years, but contributes to production after approximately 10 years.
2) The choice of injection mode impacts transport properties in kilometer-scale three-dimensional discrete fracture networks (DFN). The choice of injection mode, resident and flux-weighted, is designed to mimic different physical phenomena. Results show that after traveling through a pre-equilibrium region, both injection methods exhibit linear scaling of the first moment of travel time and power law scaling of the breakthrough curve with similar exponents, slightly larger than 2. The physical mechanisms behind this evolution appear to be the combination of in-network channeling of mass into larger fractures, which offer reduced resistance to flow, and in-fracture channeling, which results from the topology of the DFN.
3) During hydraulic fracturing millions of gallons of water are typically injected at high pressure into deep shale formations. The amount of water stored in the matrix is estimated utilizing two distinct methods—one using a two-phase model at the pore-scale and the other using a single-phase model at the continuum scale. Based on these calculations, it appears that most of the water resides in the matrix with a lesser amount in the fractures.
4) The relative importance of including in-fracture variability in flow and transport modeling of large-scale fracture networks has been under debate for a long time, since the flow in each single fracture is controlled not only by in-fracture variability but also by boundary conditions. In order to address the question of the importance of in-fracture variability, the internal heterogeneity of individual fractures is incorporated into three-dimensional DFNs. It is shown that early particle travel times are more sensitive to in-fracture aperture variability than tails of travel time distributions, where no significant effect of the aperture variations and spatial correlation length is observed.

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The Virtual Element Method in underground flow simulations

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ABSTRACT

Underground flow simulations are characterized by huge domains and very difficult geometrical configurations that usually state severe problems in mesh generation; as a consequence a large number of degrees of freedom are typically introduced. In these situations polytopal elements can introduce a wide flexibility in mesh generation. The improved flexibility can be a beneficial property that helps to reduce the number of degrees of fredom. The quite recent introduction of the Virtual Element Method [1] provides an interesting tool for the use of polygonal or polyhedral elements in underground simulations. VEM elements in 2D can be polygons with a different number of edges. DOFs on the element boundaries completely define the solution on the boundary, easily allowing the imposition of continuity conditions. Internal DOFs are used to preserve accuracy. New serendipity VEM elements were recently introduced [2] in order to keep the number of DOFs per element as small as possible preserving accuracy.
VEM elements was recently used in steady state Discrete Fracture Network simulations resorting to a new optimization based approach [3], to a mortar matching of the hydraulic head at the intersections between fractures [5], and to a totally conforming discretization on the whole DFN obtained starting from independent meshes on each fracture [6].
More complex problems can be tackled within this approach, such as - for example - transport of a passive scalar in the DFN via the introduction of suitable stabilization terms that preserve the polynomial accuracy of the VEM used, but that allow to deal with very large Pèclet numbers. Unsteady transport problems in medium scale DFN with variable transmissivity and diffusivity coefficients will be considered.
A different interesting issue regarding efficient underground simulations concerns an optimal use of the computational resources. Namely, adaptive discretizations driven by properly defined error estimates may yield a clever distribution of the degrees of freedom. A posteriori error estimates for VEM discretizations are still not completely addressed; residual based a posteriori error estimates for the steady state flow in DFNs will be presented and discussed. The computable error estimator derived is proven to be equivalent to the error between the solution of the problem and a projection of the VEM solution. Possible extensions of residual based a posteriori error estimates to the unsteady problem of the flow in DFN will also be envisaged.

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Solving the unstationary advection-diffusion problem in large scale DFNs with an optimization approach

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ABSTRACT

Discrete Fracture Networks (or DFNs) are large sets of intersecting planar polygons in the 3D space resembling the fractures in the underground. Such models are widely used to characterize the hydro-geological properties of the subsoil, and are generated stochastically starting from probability distributions of the relevant data, typically resulting in tangled networks of interconnected fractures, with heterogeneous properties.
Standard approaches, based on finite elements on meshes conforming to the intersections among the fractures, are often unsuitable for the numerical simulation of the flow in DFNs of interest for practical applications. Indeed, due to the size and to the geometrical complexity of the computational domain, the mesh generation process often results unfeasible, or produces poor quality meshes, inadequate to compute a reliable solution.
A novel approach based on a PDE-constrained formulation on non-conforming grids has been recently developed in order to effectively tackle flow simulation in large scale complex DFNs. The method suggests to split the original problem on the whole DFN in smaller problems, each written on a single fracture of the network. Then, the minimization of a cost functional, expressing the error in the matching conditions at the interfaces, is used to retrieve the coupling of the solutions on the sub-problems.
Here we use the hydraulic head distribution computed with this optimization approach to evaluate the Darcy velocity in a given DFN. The same optimization-based model is then used to solve, at each time step, the advection-diffusion problem describing the transport-diffusion mechanism of a passive scalar quantity in a network of fractures.
Numerical results are proposed on rather complex networks, also with heterogeneous hydraulic properties, highlighting the viability of the proposed approach.

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Simulation of direct/indirect hydromechanical copuling in fractured rock mass

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ABSTRACT

In a fluid-saturated rock mass, the prediction of the fluid flow sometimes requires the consideration of the Hydro-Mechanical Coupling (HMC) of pore pressures with deformation. HMC is relevant in several engineering applications in which the related physical processes are time-dependent. Wang (2000) made a distinction between direct and indirect HMC. In the first case, the coupling implies variations in the field variables (stress and pressure) of the system, without any modification of its mechanical properties. In the second case, a reduction in the pore or fracture volume results in a stiffer and less permeable material. Indirect HMC is predominant in fractured rock; in fact, under the variation of stress, fracture transmissivity can drastically change and significantly affect the flow regime in turn. For indirect HMC the prediction of the fluid flow in the near-field claims the adoption of discrete models, i.e. models in which a network of discrete fractures is superposed to the pervious/impervious matrix. The equations for the prediction are the storage equation for both matrix and fractures, the local stress balance (Navier) equations for the matrix and a stress-versus-closure equation for the fractures. The indirect coupling is condensed into an additional equation relating the fracture aperture with the mechanical (true) aperture and, consequently, with the closure. A stress-dependent coefficient f has been introduced (Fidelibus 2007; Cammarata et al. 2007). recently Souley et al. (2015) has performed experiments on fractures in granite and found a linear relationship for f.

A computer code was developed to solve in 2D this system of equations (Fidelibus 2007). For the blocks the fully coupling of storage and Navier equations is managed by resorting to an integral equation numerically approximated by means of the Boundary Element Method (BEM), whereas the diffusion equation in the fractures is dealt with the Finite Element Method(FEM) and a Galerkin weighted residual procedure. Finally, the fracture stress-versus-closure equation is directly rendered in algebraic form through spring-like equations. A time-marching process is implemented leading to an algebraic system where the right-hand side vector is built based on the collected solutions of the previous time steps. The technique requires the meshing of the fracture network only. With this scheme, fully coupling is ensured for both matrix and blocks, thus the Mandel-Cryer effect can be simulated. More relevant is the capability of the code to simulate the effect of the drastic change of fracture transmissivity when normal effective stress is modified by a fluid injection or a stress release due to an excavation. In Figure 1 the results of the simulation of a fluid injection in a single conductive fracture are reported as typical results that can be obtained (Cammarata et al. 2007).

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Wicking of liquid nitrogen into superheated porous samples

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ABSTRACT

Evaporation in porous elements of liquid-vapor separation devices is an undesired effect for vapor-free cryogenic propellant delivery to the spacecraft engines [1, 2]. On that account, the capillary transport of a cryogenic liquid subjected to evaporation needs to be understood and assessed. We investigate wicking of liquid nitrogen at saturation temperature into superheated porous media. A novel test facility was built to perform wicking experiments in a one-species system under pre-defined non-isothermal conditions. A setup configuration enabled to define the sample superheat by its initial position in a stratified nitrogen vapor environment inside the cryostat. Two experimental cases with regard to the sample superheat value were examined. Simultaneous sample weight and temperature measurements indicated a wicking front velocity during the imbibition. The mass of the imbibed liquid nitrogen was determined varying the sample superheat, geometry and porous structure. To the author's extent of knowledge these are the first wicking experiments performed with cryogenic fluids subjected to evaporation using the weight-time measurement technique. A one-dimensional macroscopic wicking model describes the process theoretically. Results show that the liquid loss due to evaporation at high sample superheats leads to only a slight imbibition rate decrease. However, the imbibition rate can be greatly affected by the vapor flow created due to evaporation that counteracts the wicking front propagation and significantly slows down the process.

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Coupled Radiation-Conduction Heat Transfer in Participating Macroporous Media

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ABSTRACT

Porous media are used and studied in many different fields due to their interesting and versatile morphological characteristics and transport properties. Besides the presence of different length scales, the coupling of physical phenomena, such as different modes of heat transfer, fluid flow and chemical reactions render their study most challenging. Understanding the coupling of the relevant physical processes is crucial when designing and optimizing devices such as heat exchangers or radiation absorbers.
Often the structure of porous media is complex and it is not possible to resolve the full geometry in practical applications. Volume averaging methods (VAMs) are instead used. VAMs reduce the complexity of the problem by deriving volume averaged conservation equation for the various components in the media, applicable throughout the domain. The volume averaging process gives rise to closure problems, resolved by introducing effective transport properties. These effective properties are derived from the morphology of the porous medium, the interface boundary conditions, and the bulk properties of the different phases. If various modes of heat transfer are considered, coupling terms will appear in the volume averaged equations, introducing additional effective properties that are not present when each mode is treated separately [1].
We developed a numerical model to account for steady state, coupled radiative and conductive heat transfer in two-phase porous media consisting of one transparent, stagnant, fluid and one participating, solid phase. The radiation transport is calculated by solving the radiative transfer equations in the stagnant fluid phase and the semi-transparent solid phase by using a path-length based Monte Carlo method. The obtained radiative flux was then incorporated as a source term into the steady state energy conservation equation and solved by finite volume techniques. The coupling was achieved by iteration, thus ensuring consistency between the radiative flux and the temperature field when convergence is reached and coupling of the two modes of heat transfer.
The method was validated using simplified geometries and analytical results and was subsequently applied to three-dimensional morphologies. The effects of coupling were quantified for different geometries, material properties and boundary conditions. An estimate of the accuracy of the use of one apparent conductivity, incorporating the effects of conduction and radiation for both phases, was given for the various conditions studied.

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Modeling of coupled conductive and radiative transfer within fibrous semi-transparent media at high temperature

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ABSTRACT

Oxides like alumina Al2O3 or zirconia ZrO2 which are refractory materials with a weak thermal conductivity. Felts composed of fibres of these oxides are candidates as insulating materials at high temperature. In these very porous materials at high temperature radiation transfer, generally coupled with other heat transfer modes, is often predominant. Furthermore, a complex morphology, a possible anisotropy, edge effects, the semi-transparency of a phase and the non-Beerian behaviour of these materials make it difficult to determine their radiative properties with classical methods.
A statistical approach is based on the complete characterisation of extinction, absorption and scattering with statistical distribution functions, which allow the Beerian behaviour of a medium to be assessed (or not) [1]. In the general case, radiation transfer is computed from a Generalized Radiative Transfer Equation (GRTE), in which the absorption, scattering and extinction coefficients are replaced by the associated statistical functions [2].
In the present work, the effective heat transfer properties of models of oxide felts are determined by taking into account a coupling of heat conduction and radiation [3]. A virtual, statistically homogeneous, two-phase fibrous sample has been built by stacking finite absorbing cylinders in a transparent gaseous volume. These cylinders are dispersed according to prescribed distribution functions defining the cylinder positions and orientations. Cylinder overlappings are allowed.
The radiative distribution functions have been accurately determined with a Monte Carlo method. Whereas the gaseous phase exhibits a Beerian behaviour, the fibre phase is strongly non Beerian. The integration of the GRTE allows thus the radiative power field deposited within the fibrous material to be determined.
The model of conduction transfer is based on a random walk method, which accounts, without complex meshing techniques, for the orientations and overlappings of the fibres of this complex morphology. The simulation of Brownian motion in fibres allows the energy equation to be solved. The idea of the method is to characterize the temperature in an elementary volume by the density of walkers, which roam the medium. The problem is governed by boundary conditions; A constant concentration (or a constant flux) of walkers is associated with a fixed temperature (or flux) [4].

This study is concluded by a discussion on the thermal insulation efficiency of such a material in different configurations (effect of the porosity, the dispersion of the orientation, the optical index, the absorption coefficient and the thermal conductivity of the fibres).

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High temperature reactivity of porous chars

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ABSTRACT

NASA's state-of-the-art technology in thermal protection systems for planetary entry vehicles uses highly porous carbon/phenolic composites as heat shield materials. Within this class, the Phenolic Impregnated Carbon Ablator, or PICA, has been successfully used to protect the Mars Science Laboratory capsule that delivered Curiosity to Mars. An ongoing effort is devoted to improve the modeling of PICA ablation under entry aerothermal conditions, and to obtain high-fidelity predictions of MSL flight data. Dedicated laboratory experiments are implemented to provide quality data on material properties and validation test cases.

The response of a phenolic-impregnated carbon ablator during entry involves complex, coupled phenomena. Pyrolysis decomposition of the phenolic phase produces gases that are transported within the porous medium and interact with the carbon fibers. Heat is transferred through conduction and radiation. The charred phase reacts with species from the incoming freestream plasma and decomposes via oxidation, and its recession is further enhanced by mechanical material removal, due to friction and shear stresses. In this study, we focus on the high temperature decomposition of the carbon fiber preform, used as a substrate for PICA. Specifically FiberForm, a rigid rayon-derived carbon-fiber preform, is exposed to oxidizing gas mixtures representative of different entry scenarios.

Results and analysis of flow-tube experiments are presented. FiberForm plug samples were placed in a tubular quartz reactor, centered in a high-temperature furnace capable of providing temperatures up 1500 K. Pure gas mixtures of O2 and CO2 were supplied to the system at controlled rates. As the gas flowed toward the sample and through the porous medium, different chemical reactions occurred, leading to the gasification of the carbon fibers. In order to characterize the decomposition rate of FiberForm at increasing temperatures, the FiberForm was weighed prior to and after testing, and correlated with gaseous products quantified using mass spectroscopy. Differential pressure measurements across the specimens allowed to quantify the Klinkenberg permeability of the virgin material, and to estimate the change of permeability in time, as the material oxidized. Changes in the microstructure due to decomposition were also characterized using scanning electron microscopy.

It is shown that in pure oxygen environment, FiberForm decomposed according to the C(s)+O2?CO2 reaction at low temperatures and C(s)+1/2O2?CO at higher temperatures. In a CO2 environment, decomposition of the carbon phase occurred via the Boudouard reaction C(s)+CO2?2CO. In CO2, Boudouard's equilibrium controlled the decomposition of FiberForm. While in O2 oxidation started at temperature as low as 700 K, in CO2 decomposition was observed only above 1200 K. Carbon loss in carbon dioxide was found to be about half of that measured in pure oxygen, at the highest experimental temperature (~1500 K).

Pore Network Modeling of Carbonate Acidization

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ABSTRACT

Dissolution of solid grains in a porous medium is important in many applications, such as groundwater transport, carbon storage, mineral systems, formation of geologic features, and enhancement of near-wellbore permeability in carbonate reservoirs. These systems are characterized by a dynamic rate of reactive transport and an increase in permeability as the medium dissolves. Many models for dissolution in porous media are continuum scale descriptions, but the flow, reactive transport, and subsequent increase in porosity and permeability occur at the pore scale. Thus, proper inclusion of parametric inputs is challenging. We present a novel, single-phase, 3D, predictive pore network model of dissolution for porous media in the mass transfer-limited regime. A mass transfer coefficient correlation and pore merging criterion are developed from finite element simulations that greatly improve the pore-scale physics and the predictive capability of the network. The optimal Damköhler number determined from our network simulations closely matches the optimum of 0.29 reported experimentally for limestone-HCl systems.

Evolution of the Properties of LSM-YSZ Solid Oxide Fuel/Electrolysis Cell electrodes during exposure tests

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ABSTRACT

Lanthanum strontium manganite-yttria-stabilized zirconia (LSM-YSZ) solid oxide fuel/electrolysis cell (SOFC/SOEC) electrodes are affected by several degradation phenomena during operation, which include the contamination of the active sites by volatile species released by the other fuel cell components and microstructural coarsening, separately or together depending upon the conditions. Exposure tests were performed under controlled conditions at 800°C in dry air during 3000 h to separate the effects of the contributions to the degradation during SOFC/SOEC operation. The total conductivity of the sample monitored using 4-point measurements was initially smaller than 1.0 S cm-1 and degraded with a rate of approximately 20 mS cm-1 kh-1.

Focused ion beam-scanning electron microscopy (FIB-SEM) serial sectioning imaging was performed to quantify microstructural changes in the exposed sample. 3-D stacks of 10x10x15 ?m of the pristine and aged samples were extracted for analysis. 3-D characterization started with a volume and grid independence study for selected metric and topological properties. Phase size distribution measurements showed that the LSM phase distribution is slightly coarser and less connected in the exposed sample, which further resulted in a decrease in connected triple-phase boundary length of 5 %. Pore-level simulations of fluid flow and species transport in the pore phase, and electron, ion and heat transport in the two solid phases were conducted. The results for the sample before and after exposure were implemented in a continuum composite electrode model to investigate the effects on the electrochemical performance. The results capture the low total conductivity measured, compared to the bulk electronic conductivity of LSM (approx. 100 S cm-1) and the observed degradation. Further, the ionic conductivity, diffusivity and permeability slightly increased, consistent with the observed changed in phase volume fraction and coarsening of characteristic phase dimensions.

Permeability evolution in fractures exposed to reactive flow and normal stress: Fracture sealing vs. run-away flow

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ABSTRACT

Permeability of rock fractures can increase significantly due to reactive flows that cause mineral dissolution, especially if positive feedback between flow and reaction produces channelization. Very little is understood about how permeability evolves when reactive transport is coupled with constant normal stress. Understanding this coupling is critical to predicting the migration of environmentally-relevant fluids. This study couples a two-dimensional reactive transport model with a geomechanical equilibrium model to simulate reaction, flow and elastic deformation in a fractured carbonate rock. The simulations aim to understand the effects of the spatial distribution of reactive and non-reactive minerals on fracture evolution in shales and other caprock formations. Initial fracture aperture geometries were designed to match the aperture distribution in an experimentally-fractured core of Indiana Limestone. For fractures representative of the Amherstburg Limestone and the Eagle Ford shale, mineral maps that identify reactive versus non-reactive minerals were inferred from experimental analyses, including synchrotron based XRF maps. It was found that for a fracture in a mineralogically homogeneous rock, such as the Indiana Limestone, dissolution leads to extensive erosion near the inlet, and permeability is controlled by unreacted downstream apertures. When the rock includes areas of nonreactive minerals, the fluid can flow further downstream without being buffered, leading to faster increases in permeability. Furthermore, mineral heterogeneity creates areas of contact points that do not get reacted away, leaving support holding the fracture walls apart. Simulation of reactive transport without mechanical loading will lead to overestimation about the potential for leakage through caprock fractures, as is relevant in the context of geologic carbon sequestration.

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Permeability of partially- and fully-cemented fractures

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ABSTRACT

Natural fractures are commonly lined, bridged, or fully cemented with mineral precipitates. The permeability of these fractures deviates significantly from what is typically estimated by cubic-law type models. Here we present an analysis of fracture permeability for partially- to fully-cemented fractures by combining direct numerical flow simulation techniques and multiscale imaging (i.e. scanning electron microscopy, x-ray computed microtomography) of cement structures. The permeability of natural fractures is shown to vary over orders of magnitude as a result of pore space geometry and cement structure. Fractures lined with mineral cements have permeability that is within an order of magnitude of that estimated by cubic-law type models, however, as the fracture cement lining begins to fill in the remaining pore space, the fracture permeability precipitously drops. The permeability of partially-cemented fractures that contain connected macroporosity have permeability that is similar to that of porous media due to many fracture plane contacts restricting the flow. Once the macroporosity of the fracture becomes increasingly disconnected, the permeability of the fracture becomes a function of the permeability of the cement. Once fully-cemented, overall fracture permeability is controlled by the permeability of nanoscale grain boundary channel networks within the cement. We then use the results from numerical flow simulations to construct formulations for estimating fracture permeability based on the characterization of the fracture pore space geometry and cement structure for the entire range of possible mineralization, e.g. from mineral-lined to fully-cemented.

An Investigation of Dynamic Proppant-Pack Conductivity

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ABSTRACT

The conductivity of proppant packs can play a critical role in the productivity of a hydraulically fractured well. In this paper we focus on evaluating the conductivity of propped fractures, the role of the proppant size distribution and the processes controlling fracture closing. Several factors influence the conductivity of a propped fracture. Here we investigate the influence of differential stress on proppant packs and the related impact on the propped fracture conductivity.

We combine the Discrete Element Method (DEM) and the Lattice Boltzmann Model (LBM) to investigate the effect of increasing differential stress on proppant pack conductivity. A loose assembly of variable size spherical particles with no initial contact is generated in DEM, and then compacted under a specified confining stress to generate the initial proppant pack. Differential stress is then applied and increased on the proppant pack to simulate production (draw-down) until the formation of shear band(s) initiates (proppant failure). A representative elementary volume of the proppant pack, at a given stress state, is used for fluid flow simulations. We use LBM to calculate a detailed flow field at the pore scale and evaluate the related Darcy-scale permeability. This process is repeated for increasing differential stress to simulate changing conditions during production.

By considering the geomechanics of the proppant packs, we combine permeability and fracture aperture to determine the propped fracture conductivity: We calculate the width of the fracture to evaluate the dynamic conductivity of the proppant pack during production. With increasing differential stress on proppant pack, the aperture decreases and causes further reduction in the conductivity. In particular, we demonstrate that well-graded proppant packs maintain higher fracture conductivities over a range of stress conditions that are relevant to production operations.

The proposed workflow provides an effective approach for improved analysis of production dynamics from hydraulically fractured wells, and provides a path to optimize the proppant size distribution based on expected variations in the subsurface stress field. Furthermore, accurate input to simulators, in terms of fracture conductivity tables, can be generated via the presented work flow.

X-ray micro CT for structural and compositional analysis of cores at different scales (dm -> µm)

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ABSTRACT

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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Fluid-driven crack propagation of pre-fractured porous media

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ABSTRACT

Hydraulic fracturing, as a widely used technology in the oil industry, usually occurs in the gas and oil bearing rock. Due to the complexity of the stratum, many aspects have to be considered in the relevant study. Firstly, different components in different phases exist in the stratum, which interact with each other during the fracking process. Therefore, an appropriate homogenisation method, together with a proper description of the interaction, is required for such a multi-phasic and multi-physics problem. Secondly, the evolution of cracks plays a decisive role in the fracking process, which does not only directly influences the behaviour of the solid skeleton but also results in the transformation of the flow type due to the vanishing interaction. Thirdly, the stratum is an imperfect continuum as defects and cracks have already been included before the loading process. Besides, the stratum is not initially stress-free. Experiments have already shown that both the imperfections and the initial pressure have significant influence on the crack evolution.

Focusing on the above-mentioned features, the authors present a new approach based on the phase-field theory included in the Theory of Porous Media, where an order parameter is defined as the state measure of the solid skeleton. The order parameter evolves from 0 (intact material) to 1 (cracked material) under the accumulating potential energy of the porous solid caused by positive eigenvalues of the strain tensor. By including the order parameter in the constitutive equations, the resistence of the solid skeleton is gradually degrading in the direction of the eigenvector related to a positive eigenvalue. In the meantime, the interaction term also vanishes, and the frictional extra stress of the fluid arises. This transforms the Darcy filter flow to the Navier-Stokes flow. In conclusion, a model is set up to demonstrate the fracking process under prestresses and precracks. Different settings of prestresses are applied to the model, and the results are compared with relevant experiments.

Temperature Effect on Drying Kinetic in Porous Medium

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ABSTRACT

The evaporation is a common important process for many industrial and engineering applications such as soil salinisation (relating to the excess accumulation of salts in soil), paper industry, building material, pharmaceutical applications, geological carbon storage and food processing [1, 2, 3, 4, 5, 6].The drying kinetic behavior has three main distinguished regimes including (a) constant rate period, (b) falling rate period, and (c) receding front period [7]. The drying dynamic depends on the interface between the external and internal mass transfer during the evaporation and also depends on the drying air characteristics such as air temperature, relative humidity and airflow velocity.

The specific objective of this study was to assess the drying behavior of the Bentheimer sandstone under different air temperatures including 30 oC, 60 oC and 80 oC. The assessment was performed under zero air relative humidity and negligible airflow velocity.

In this study, a series of experimental investigations for the drying rate evolution with time was performed. We used Bentheimer sandstone rocks sample with mean grain diameter of 0.23 mm. The investigations were performed in diffusive drying condition (no flow was imposed) using sand-filled cylindrical column with diameter of 6 mm and 20mm length. Also, a baseline Micro-CT image of the surface of Bentheimer saturated with water at 6μm voxel size was performed.

Based on the dry-out experimental investigations, it was evident the effect of increasing the temperature on drying rate as shown in Figure 1. The period of constant drying rate (CRP), as is typically the case for porous media, is either very small or does not exist at all for all high air temperature case tested as shown in Figure 2. The value of average water saturation decreases rapidly, with consequent increase of the drying rate, when temperature increased. Therefore, it can be concluded that during the constant drying rate (CRP) is an atmospheric controlled process.

Based on the Micro-CT image (see Figure 3), it was demonstrated that initially, the big pores started drying out first leaving a thin film of water in the pores, however, due to capillarity flow; the small pores were still filled with water. After 8 hours of drying out process of the Bentheime sample, the transition period was reached where the big pores are completely dried out and the small pores are mostly dried out as shown in Figure 3 (c).

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Numerical investigation of shale gas simulation in fractured porous media using single continuum vs. dual continuum approaches and the effect of accounting for stress-affected deformation

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ABSTRACT

The Dual-porosity Dual-permeability (DPDP) model was commonly used in simulating flow in fractured porous media. However, it was difficult to control all the parameters in detail or to see the exact flow behavior through fracture networks using the DPDP model. This was caused by the fact that the DPDP model considers the whole domain in one continuum as a matrix and in the other continuum as a fracture without any consideration for the actual fractures network shape; then the connection between the two continuums is made by a transfer term that appears in both continuum equations. This kind of dealing with the domain is almost as if the two continuums are occupying the same domain in the DPDP model assumption. This is not consistent with the actual reservoir properties in fields.

In this paper, we explore the possibility of specifying the exact positions and sizes of the fracture networks in the same dimension as the matrix blocks dimension in a single-continuum reservoir model. In other words, for example, if we consider 2D matrix blocks, we specify the positions and sizes of the fractures in 2D too. We called our simulation the Single-Domain Fracture Model (SDFM) throughout the paper. Using the SDFM, we explore the exact flow behavior through the fracture networks using different fracture networks shapes. SDFM consists of a single equation for a single-continuum unlike the DPDP model that consists of two equations each for one of its continuums and both equations are coupled by a transfer term as we mentioned before.

We also mimic the DPDP configuration assumptions used by Warren and Root [1] and many other authors [2-5]. Since both models, DPDP and SDFM, are simulating the same configuration, we compare the results of both models using the same parameters to see how close the results are to each other and what might be causing the behavior difference for each model. We also perform some numerical experiments on the two models such as the effect of changing pressures, porosities…etc. Finally, we investigate the stress affected rock deformation in the DPDP and SDFM models and its effect on the permeability and production rate.

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A general and flexible methodology to model dependencies in discrete fracture network simulations using Bernstein copula approach

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ABSTRACT

In many natural fractured porous media, such as aquifers, soils, oil and geothermal reservoirs, fractures play a crucial role in their flow and transport properties. An approach that has recently gained popularity for modeling fractured systems is the Discrete Fracture Network (DFN) model. This approach consists in applying a stochastic boolean simulation method, also known as object simulation method, where fractures are represented as simplified geometric objects (line segments in 2D and polygons in 3D). One of the shortcomings of this approach is that it usually does not consider the dependency relationships that may exist between the geometric properties of fractures (direction, length, aperture, etc), i.e., each property is simulated independently.
In this work a very general and flexible methodology for modeling such dependencies applying a copula theory approach is introduced. In particular, a non-parametric model using Bernstein copulas for direction-length-aperture fracture dependency in 2D is presented. The application of this method is illustrated in a case study for a rock sample from a naturally fractured carbonate formation.

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Experimental study on fluid-driven cracks and backflow in an elastic matrix

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ABSTRACT

A laboratory scale experiment was developed to study the physical mechanisms of fluid driven fracture and the backflow from elastic reservoirs. When a pressurized fluid is injected into a gelatin matrix, which is elastic but brittle, the fluid generates a fracture that grows along a plane and forms a fluid-filled disc-like shape. Once the injected fluid is exposed to the atmospheric pressure, the elastic relaxation of the reservoir drives the fluid flows backwards (backflow) towards the original source. We measure the crack shape as a function of time, which has not been studied before, for both the fracturing and backflow processes, and investigate the influence of different experimental parameters such as the injection flow rate, Young's modulus of the matrix and fluid viscosity.

In the fracturing process, the elastic stress in the matrix surrounding the crack is balanced by the viscous stress in the fluid flow and the toughness-related stress. A pressure ratio is defined to estimate the relative importance of toughness-related stress to viscous stress. (ref. 1) Based on this pressure ratio we're able to tune the experimental parameters to explore both the viscous and toughness dominated regime. We find that the crack radius R(t) increases with time according to a power law with slightly different exponents for the viscous- versus toughness-dominated regimes. For both regimes, the rescaled experimental data at long times for different parameters collapses based on the scaling arguments available in the literature. (ref. 2-3)

Next, we measure the time evolution of the crack shape for the fracturing process in both the viscous- and toughness-dominated regimes, and the backflow process. The rescaled crack shapes collapse at longer times and show good agreement with the scaling arguments.

The gelatin system provides a useful laboratory model for further studies of fluid-driven cracks, which has important applications such as hydraulic fracturing.

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Multiscale Coupling of Image-Based Pore-scale Flow Models

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ABSTRACT

Increasingly, imaging technology allows porous media problems to be modeled at a very fine, microscopic scale. However, the physical domain size required to be representative of the media can prohibit comprehensive micro-scale simulation. Therefore some hybrid, or multiscale, approach is necessary to overcome this challenge. A new multiscale modeling methodology has been developed which can be used to solve practical porous media flow problems and to better understand the interaction/dependence of phenomena occurring at different microscopic scales. This approach employs coupling of microscopic simulations (fluid streamline scale) with coarser pore-scale models. Network modeling is a common pore-scale technique which employs rather severe assumptions, making it more efficient than direct numerical simulation of the equations of motion, and is thus able to operate over much larger length scales. However, microscopic features of the medium are lost in the discretization of a material into a network of interconnected pores and throats. In contrast, detailed microstructure and flow patterns can be captured by modern meshing and direct numerical simulation techniques, but these models are computationally expensive when applied over large domains. A multiscale technique has been developed that couples the two types of models, taking advantage of the benefits of each. Specifically, an image-based physically-representative pore network model is coupled to an FEM solver that operates on unstructured meshes capable of resolving details orders of magnitude smaller than the pore size. In addition to allowing simulation at multiple scales, the current implementation couples the models using a machine learning approach, in which results from the more accurate FEM model are used by the network model to learn specific modeling parameters. This talk will present examples of the model that operate on real porous materials (imaged by synchrotron X-ray computed tomography) and artificial computer-generated materials. Examples are given that illustrate the simulation of sub-pore-scale features and fluid mechanics as well as the improvements in network modeling enabled by machine learning from the more fundamental modeling.

The Wilcox formation: a case study for integrating pores from multiple length scales

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ABSTRACT

The complex texture of the Wilcox tight gas sandstone formation makes an excellent example of a geomaterial whose a priori prediction of transport properties relies on a correct and cost-effective model that integrates pores from multiple length scales. The nanometer to micrometer scale range in pore sizes of this medium imposes uncertainty in the capturing of the pore space in a single imaging modality with a large enough field of view. Even with an image that has captured the entirety of the pore space, the increase in number of voxels due to the existence of this range of scales in close proximity, results in costly computations. These challenges make a direct solution of any flow constitutive equation in the pore space unfeasible.

Pore-network models, the representation of the pore-space via a ball (pore) and stick (throat) ensemble, mitigate the computational cost that results from explicitly voxelizing the pore-space. In this presentation, we discuss the reconstruction of multiscale network models as our attempt to integrate the pores from multiple length-scales in a cost-effective single-entity network model.

Two schools of thoughts are employed in our approach: a process-based method and an image-based method. In the process-based method, petrographic analyses using transmitted light microscopy are used to infer the diagenesis of the rock. These diagenetic steps are quantitatively followed to reconstruct the porous medium. The nanometer scale pores are resolved using scanning electron microscopy and information from them is further gathered by conducting nitrogen sorption measurements. The micrometer to nanometer scale pore structure is represented via a multiscale network model in the final step. In the image-based method, a micro-CT image of the sample is taken and a multiscale network model is extracted based on skeletonizing the micrometer size pore space and mapping nanometer scale clusters of micropores to the unresolved porous areas. The drainage capillary pressure curve of the rock is predicted using these two methods and the results are compared with mercury injection measurements. The fidelity of the two approaches in predicting the single and two-phase flow properties is investigated.

A comparison of a free energy MRT Lattice Boltzmann method for two-phase flow with a fully dynamic network model

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ABSTRACT

Predicting fluid behaviour during imbibition is still a challenge for network models [1]. This is due to the nature of the imbibition flow mechanism in porous media as a result of snap-off of the non-wetting phase at constrictions. Recently, the Lattice Boltzmann methodology has found applications in two phase flow simulations in porous media and has the advantage of local computation of fluid properties [2]. In this study, we take advantage of the microscopic/local nature of Lattice Boltzmann numerical models as well as its accuracy to investigate multiphase fluid behaviour in porous media.
The Lattice Boltzmann model was validated against benchmark cases for Poiseuille flow and for a lid driven cavity flow in three dimensions. We implemented a multi-relaxation time approach to simulate two phase flow and validated our model against Laplace's. Simulations were carried out for a range of wettabilities and the static contact angle determined for a two phase carbon dioxide water system. Numerical Simulations were the carried out on Bentheimer sandstone to study the effect of variations in rate of fluid injection on relative permeability using different boundary conditions. We investigate the effect of grid discretisation and initialization techniques for our flow simulations.
Results of our numerical study are compared with those of a dynamic network model; first for a range of simple geometries and ultimately for Bentheimer Sandstone for different contact angle and flow rate scenarios.

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Assessing the influence of microporosity on imbibition in complex pore structures with multi-scale pore network models

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ABSTRACT

Understanding the relative permeability behavior of complex geological materials during imbibition is an important challenge in e.g. petroleum engineering, environmental engineering and CO2-sequestration. While image-based pore network models have helped to understand how the pore-scale properties influence this behavior, specially adapted multi-scale models are needed to perform such simulations on rocks with wide pore size distributions. In previous work, we have developed a multi-scale image-based pore network model, which takes unresolved microporosity into account by adding special links (micro-links) with upscaled microporosity properties to the classical network description (pores and throats) [1]. Here, we present rules to simulate imbibition in such networks under different wettability scenarios.

Compared to drainage, the filling sequence during imbibition is more complex, as snap-off and cooperative pore filling have to be taken into account. In our model, the saturation and fluid conductivities of the microporosity at each point in the simulation are encoded in capillary pressure and relative permeability curves which are provided as input. Thus, an adequate network description of the microporosity is required to assess these curves under the prevailing wettability conditions. This network description can for example be obtained by performing high-resolution imaging experiments on the microporosity.

To describe the filling sequence of the multi-scale network as a whole, the connectivity of both fluid phases (e.g. oil and water) in the microporous links is taken into account. Macropores can be filled with the invading fluid through neighbouring microporosity if it percolates through the microporosity. During waterflooding in the water-wet case, the invasion capillary pressure at which this happens is generally controlled by the geometry of the macropore. During waterflooding under oil-wet conditions, the invasion capillary pressure is instead controlled by the microporosity, and a percolation theory approach is used to determine through which micro-links water percolates first. Furthermore, microporosity can also provide an escape path for the defending phase if this phase percolates through it. We thus also take the defending phase's connectivity into account at the prevailing capillary pressure, which can affect the network's trapping behaviour.

In this work, we show how quasi-static, multi-scale pore network models can be used to incorporate information from multiple scales, and we illustrate how this approach can be used to investigate the influence of microporosity on relative permeability and resistivity index behavior during imbibition. The validity of the model is tested by comparing results to network models with individual micropores [2] and by treating networks extracted from micro-computed tomography scans of rocks with complex pore geometries (e.g. carbonates).

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A new multi-threshold method for multi-scale digital rock image segmentation and upscaling in tight sandstone reservoir

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ABSTRACT

Digital rock image segmentation is an important prerequisite for the studies of microscopic pore structure and porous flow mechanism. Rather than divide image explicitly into pore space and grains as in traditional one threshold segmentation, multi-threshold segmentation enables upscaling by considering the interconnected matrix as these matrix may represent an averaged grayscale of a region of micro pores and grains.

Due to the trade-off between computer tomography scan (CT scan) resolution and sample size, multi-scale CT scans and a digital rock upscaling method is applied in order to characterize the multi-scale pore structure in heterogeneous rocks. Figure 1 shows a general two-scale upscaling approach for a carbonate sample. To produce representative predictions for the entire rock sample, this procedure use a high resolution CT-scanned subsample of a selected representative elementary volume (REV) to represent matrix voxels in large-volume coarse scale image.

In more complex tight sandstones, however, it is difficult to extract an REV-subsample that contains pure matrix – it always includes unwanted macro grains and macro pores, as illustrated in Figure 2. This leads to partial double-accounting of macro grains and macro pores when upscaling the matrix properties, calculated on the subsample, to the coarse-scale volume.

In this paper, we present a novel three-step upscaling approach to more accurately merge a high-resolution image into a low resolution image. In the first stage, a coarse-scale, gray-shade CT image is segmented into macro grains, matrix volume, and macro pores by 2 thresholds. Macro grains and macro pores are segmented rather safely to avoid voxels where interconnected matrix may apply. In the second stage, we obtain fine scale image of a selected subsample by high resolution CT scanning. As stated above, this subsample inevitably contains unwanted macro grains and macro pores. We use a watershed algorithm to segment this subsample into pores and solid phase. Then we calculate the Euclidean distance of all voxels in the 2-phase subsample image to its nearest phase boundary. Voxels that have distance numbers larger than the true spatial resolution (TSR) of the coarse CT image are recognized as macro pores or macro grains – all voxels with distance numbers smaller than the TSR are micro pores and micro grains. The result of this procedure is a segmented 4-phase image consisting of micro pores, macro pores, micro grains and macro grains. Note that since the edges of macro pores and grains are divided into micro pores and grains, the connectivity of micro pores is kept. In the final stage, we calculate the properties of micro pores and micro grains in the subsample and merge the results into coarse scale image. For example, the total porosity could be calculated from the macro pore and micro pore percentage directly, the absolute permeability could be calculated by incorporating fine scale image property into coarse scale image.

This new method solves the subsample selection problem in highly heterogeneous tight sandstone samples, provides reasonable linkage between separated macro pores in coarse image, and lays a solid foundation for two-scale and three-scale digital rock upscaling in tight sandstone reservoir.

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An analysis of NMR flow propagators for heterogeneous materials using micro-CT imaging

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ABSTRACT

Flow propagators have been frequently used in porous media characterization and to characterize fluid flow within. Scheven et al. [1], Codd et al. [2] and others measured flow propagators in various media and discussed how dispersion or other effects like relaxation and internal gradients affect its shape by changing flow behaviour. In addition, numerical simulations were used by many researchers to match their measurements [3].
However, these works mainly focused on homogeneous media like beads pack and clean sandstones. Heterogeneous cores were also studied by a few groups, but their interpretations lacked quantitative analysis of how pore geometries affect fluid transport which shapes the flow propagators.
In this work we consider the flow propagator as tool to partition disordered materials in terms of the local environment. In particular, we are interested in the connectivity of local regions as well as their individual properties.
We introduce the concept of a local propagator, which refers to a propagator measured over a short encoding interval such that regions of different character do not significantly couple. In this regime it is assumed that the averaged propagator measured via NMR is the weighted sum of the propagators of the individual regions. At longer dispersion times the local propagators will show effects of mixing before eventually coupling fully.
Here we use bead packs to represent different sample regions. For the analysis we define two different regions of the sample, namely micro- and macro-porous regions. These regions are realised experimentally by 0.5mm diameter beads and 1.5mm diameter beads, respectively. The simulations are carried out with embedded region labels. Dispersion is then modeled using a random walk on top of a velocity field derived with a lattice Boltzmann method [3,4]. The region labels are used to track individual random walks over time.
We compare the average propagator accessible via NMR to the simulation [5] results for a range of different dispersion times and Peclet numbers and find good agreement. Given this, we then use the numerical simulations to compose the average propagator into four categories, namely two ``pure'' propagators which include only averages over the micro-porous and macro-porous regions, as well as ``mixed'' propagators capturing the cases of random walks crossing region labels. The measured average propagators are thus decomposed into their respective mixed compartments as function of mixing time. We quantify the effect of this mixing with respect to both the sphere packs considered as well as random media and relate the mixing modes to the level of disorder of the microstructures considered.

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Salt Contaminant Distribution inside PEFC GDL Analyzed from X-Ray Tomography

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ABSTRACT

Recent findings related to cationic impurities in Polymer Electrolyte fuel cells (PEFC) have found that mass transport issues can occur in conjunction with electrochemical losses experienced by cationic contamination of NafionTM [1]. In a PEFC airborne contaminants are required to pass through the gas diffusion layer (GDL), prior to interacting with the catalyst layer and membrane. Both ex-situ [2] and in-situ [3] cation contamination experiments have shown that the hydrophobicity of the GDL plays a critical role in generating a barrier to the cation poisoning of the catalyst layers and membrane.

This work examines the cationic salt distribution, using micro-XCT, inside the cathode GDL in the case of a PEFC generating 200mA/cm2 while a constant 5ppm calcium sulfate impurity concentration, dissolved in water, was injected into the cathode air flow. Testing showed a significant increase in voltage decay rate, while, following tear down of the cell after the end of test, it was found that significant salt deposits were present on the GDL surface (Figure 1) facing the flow field. Additional salt deposits had clogged the outlet port of the cathode flow channel resulting in a rapid end to cell testing.

Imaging of the cathode GDL using Xradia's mirco-XCT-400 system showed significant salt deposits under the surface that contributed to increased mas transport resistances in the GDL during operating. Additionally, tomographs obtained at different locations throughout the cathode GDL showed two distinctly different precipitation patterns. Initially, near the inlet as shown in Figure 2, the salt deposits appear uniformly distributed, with no preferential precipitation location. In contrast, towards the center and outlet of the cell, a heterogeneous precipitation pattern was observed (Figure 3), where salt deposits were seen centralized under the rib of the flow plate. Analysis of the water transport through the cathode linked the localized type of precipitation observed to the local water concentration. It was found that in regions with the highest levels of GDL saturation near the inlet, the homogeneous distribution occurred, while as the water concentration decreased towards the vapor saturation concentration in the middle and outlet of the cathode, the under rib precipitation pattern was preferentially generated.

Tomographs were exported into Matlab, which calculated the in-plane and through-plane porosity distributions to understand the reduction in porosity incurred with the salt deposits. In-plane analysis confirmed both the homogeneity of the first precipitation pattern near the entrance region, and the preferential precipitation observed in the center and exit of the cell. Analysis of the through-plane distribution patterns shows that salt deposits are primarily precipitated in the region nearest the flow field, as the GDL prevents the liquid water with dissolved cations from penetrating towards the MEA. The heterogeneous precipitation can be explained through wicking of the liquid phase under the ribs

which upon evaporation, lead to the dissolved salts exceeding the saturation concentration and precipitating out. Comparison with a non-contaminated fresh GDL shows that the salt buildup in the GDL can result in a porosity reduction of up to 27% locally.

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Understanding Evaporation in Fuel-Cell Gas-Diffusion Layers with X-ray Computed Tomography

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ABSTRACT

Effective water-management is essential for the performance and stability of polymer-electrolyte fuel cells (PEFCs). In these devices, heat and mass-transport are coupled due to two-phase transport of water, where, at higher operating temperatures, liquid water produced by electrochemical reaction at the cathode evaporates in the various fuel-cell porous media and is removed into the gas flow channel in vapor form. Understanding such evaporation phenomena in a mixed wettability, porous carbon gas-diffusion layer (GDL) is necessary due to its impact on overall fuel-cell water management. In the limited number of previous studies on this topic, evaporation rates in mixed-wettability GDLs were measured as a function of liquid-water saturation [1-2]. These measured rates could not convey information about the intrinsic evaporation rate due to lack of knowing the surface area of liquid water inside the GDL, or whether these evaporation rates are kinetically or diffusively limited. Here, liquid-water evaporation rates in GDLs were measured in-situ using synchrotron X-ray computed tomography (CT). X-ray CT allowed visualizing the evaporating water-front location and surface area during evaporation experiments. To isolate contributions of convective, diffusive, and kinetic contributions to the overall evaporation rate, we systematically varied experimental parameters and explored their interaction through mathematical modeling. A three-dimensional computational model with direct meshes of liquid-water evaporation fronts from X-ray CT studies supplemented the experimental studies to characterize the geometry dependence, and to elucidate diffusive and kinetic limitations of the evaporation phenomena in porous media.

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Investigation of Porous Structure Formation of Catalyst Layers for Proton Exchange Membrane Fuel Cells and Its Effect on the Performance

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ABSTRACT

In proton exchange membrane fuel cells (PEMFCs), catalyst layers (CLs) are one of the most important components to achieve both high performance and cost reduction. Synthesizing CLs and catalyst coated membrane (CCMs) has been gathering much attention for optimization to satisfy these demands. We have focused on the fabrication process and investigated effects of the fabrication conditions on the porous structure of the CLs [1-3]. The fabrication process consists of a blending of the materials and solvents to form a catalyst slurry, applying the slurry on a substrate by doctor-blading, drying to form the porous structure evaporating solvents, and decal transfer onto the polymer electrolyte membrane by hot pressing. In this study, we especially focused on the drying and hot pressing to modulate porous structure. Hot-pressing pressure can affect the structure by compressing the pores. The drying is the other key process to control porous structure because solvents evaporate and materials gather with large volume reduction and form the porous structure during the process. To clarify the effects of these fabrication conditions on the resultant porous structure, nitrogen physisorption measurement of the CCMs were conducted and evaluated porosity and pore size distribution. Performance evaluation was also conducted to clarify the effect of the fabricated porous structure on the cell performance.

The hot-pressing pressure was varied from 0.5 to 10 MPa, and CCMs were fabricated keeping the other fabrication conditions and material components constant. Porosity obtained from the physisorption measurement decreased with the increase of the pressing pressure. The peak position in pore-size distribution was also decreased from 70 to 30 nm. Drastic voltage drop appeared in the polarization curve when the hot-pressing pressure was over 2MPa. This can be because of the decrease of the porosity and the pore size in the CLs. However, we can't identify these effect respectively because the porosity and pore size can't be controlled independently by hot pressing.

For the further control of the porous structure and evaluate the effect of porosity and pore size independently, we tried structural control in the drying formation process. Temperature and humidity in the drying were controlled. Weight variation was measured by using an electric balance to determine drying time. The temperature was 20 or 40degC, and humidity was 0 or 80%RH. The determined drying time was varied from 8 to 45 min. The porosity and pore-size distribution were measured. The porosity of the CL with longer drying time (20degC and 80%RH) showed slightly lower than the others, although all of the peak positions in the pore-size distribution was almost the same. The polarization curve of the CCMs was obtained and showed almost the same curve. The porosity difference by the drying time is almost the same with the difference by the hot-pressing pressure from 2 to 5MPa. The two polarization curve of hot-pressing parameter showed the significant difference, although that of drying parameter didn't show the difference. This means that the pore size in the CLs is the more significant factor which affects overpotential in the polarization curve than the porosity.

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GDL Wettability Changes in Cationic Contamination and Mitigation for PEFCs

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ABSTRACT

Cationic impurities on performance loss are investigated by incorporation of foreign cation into the MEA in a form of salt solution. The effect of cationic contamination and mitigation to gas diffusion layer (GDL) properties has been studied by an ex-situ soak method and an in-situ injection through the cathode inlet using a nebulizer [1-3]. Foreign cations from air pollutants and fuel cell metallic components can change surface properties of GDL by depositing on the carbon fibers, resulting in mass transport losses and water management issues from changes in hydrophobicity of the catalyst layer and the GDL. Wetting property changes of the contaminated GDL and micro-porous layer (MPL) were tested using a force tensiometer, which is measured in the sample mass changes by contacting and penetrating the liquid. The three-phase boundary contact of solid-liquid-gas onto the GDL is moving during the fuel cell operation, therefore dynamic contact angles were measured in advancing and receding angles by Wilhelmy balance method. Internal contact angles of the GDL to water also were measured by the absorption method which is measured mass changes during the rise of liquid into the pores of the porous media due to capillary action developed by Washburn. Figure 1 (a) shows water submersion cycles of the wetted surface force acting on GDL for the as-received and after soaking in DI water and CaSO4 solution at 80°C for 100hr. The contaminated GDL shows the lowest contact angle in both immerging and emerging to the liquid. The GDL wettability after soaking in the DI water was also reduced by aging effects in the hot water for 100hr. After the cationic solution injection test, the visual observation of CaSO4 salt deposits onto the GDL is shown in Figure 1 (b), such salt deposits can absorb more water during the wetting force measurement resulting in the lowest contact angles. Figure 2 shows wetting processes for the dynamic contact angle while measuring the force on the sample due to wetting.

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X-ray Tomographic Microscopy Images of Gas Diffusion Layers – Segmentation Procedure and Evaluation

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ABSTRACT

X-ray tomographic microscopy (XTM) images provide a unique insight into structure of gas diffusion layer (GDL) materials used in proton electrolyte fuel cells (PEFC). The resolution of few micrometers enables to resolve the fine microstructure formed by fibers and binder.

Steady state operando XTM images are used as input for simulations and provide information on how compression or saturation influences the gas transport in the GDL [1]. The development of fast tomography (i.e. to the sub-second range [2]) to reduce dose to the materials or to image transient phenomena in fuel cells requires a trade-off with image quality. The same trade-off exists for laboratory micro-CT installations, though on a different time scale. There, a reduction of scan time from one or two hours to a fraction of an hour would enable much higher sample throughput. Therefore, improved segmentation procedures are needed and their feature detectability has to be verified.

The GDL is typically segmented into two distinct phases: a void and a solid phase using some threshold methods [1-4]. The solid phase usually combines fibers and binder because of the low contrast between these two materials. Choice of the threshold value is an important step to ensure an optimal segmentation. Different automatic procedures exist but it remains difficult to evaluate their precision.

In order to judge the quality of a segmentation workflow, images with known structure and defined signal-to-noise ratios (SNR) are required. For this noise in GDL images need to be artificially generated in a controlled manner. A method based on differentiated voxel value assignment depending on the phase (void, solid) has been developed. Further types of noise can be added, to account for i.e. beam fluctuations or other noise related to image acquisition. The result of a segmentation workflow applied to the generated noisy image can then be compared to the original binary image for qualification of the segmentation procedure.

The production of images with known structure and defined noise, as well as the evaluation of different segmentation procedures will be reported. The qualification of segmentation workflows will allow optimizing for the experiments the minimum SNR and thus the best possible time resolution with confidence in the result after segmentation. The prognosis of the approach will be compared to real CT data of a GDL sample acquired with different scan settings which may result in reconstruction artefacts that might not be represented by the artificial data noising.

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Land-Channel Geometry in Proton Exchange Membrane Fuel Cells

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ABSTRACT

Land-channel geometry is necessary for proton exchange membrane fuel cells to transport electron and at the same time to transport reactants/products. However, this configuration causes the difference in transport distance between the flow channel to the catalyst layer through the porous transport layer, and results in the non-uniform distribution of various factors, such as species concentration, current generation, and rate of degradation [1]. In order to understand the effect of land-channel geometry, a small-scale segmented cell with about 300-micron resolution was developed [2]. The obtained results about the current density and proton conductivity distributions at various operating conditions clearly revealed the effect of the transport distance difference between under the land and under the channel. The data were further analyzed to quantify the localized ohmic and activation overpotentials [3][4]. The estimated oxygen transport distance is longer than simple geometrical transport length.

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Limiting Current Density of PEM Fuel Cells Based on Gas Permeability of Porous Transport Layers Using Pore Network Modeling

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ABSTRACT

Water transport in the porous transport layers (PTL) plays an important role in the efficient operation of of polymer electrolyte fuel cells (PEMFC). Too much water as well as dry operating conditions result in decreased fuel cell performance. In the current study thermal and mass transport in PTLs is studied using a pore network model. The network consists of coupled pore phase and solid phase model. The characteristics pore size distributions for the PTLs are obtained from porosimetry tests. Flooding of the PTLs may occur if the water generated during the cell operation is not removed at an optimal rate. The flooding results in the blockage of paths of of reactant gases to the reaction site thereby reducing operational performance. The maximum current densities at which the PTL flooding occurs at different operating conditions are estimated using the calculated permeability of different PTLs. This can be used to study the relative performance of different PTLs under different operational parameters.

Estimation of Effective Cake Filtration Simulation Parameters from Resolved Filtration Simulations

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ABSTRACT

The cake formation on the filter media scale is simulated by the following steps: First, a stationary flow through the filter media is computed. Then, particles are introduced and moved according to the friction of the fluid, inertia and Brownian motion. Filtered particles are deposited on the fibers. They change the flow field for the later particles, which can then be caught either by the filter material or the previously deposited particles. In this way, a filter cake forms. The whole process can be simulated using the FilterDict module inside the GeoDict software.

Two cases can be distinguished for monodisperse particles that dependent on the relation between particle size and the resolution of the computational grid (voxel size):

1. If the particle diameter is large enough that a particle is resolved by the computational grid, a deposited particle fills several grid cells (voxels), turning them from pore to solid. Thus, the flow through the filter cake can be modeled with the Stokes equation. In this way, the solidity of the cake and flow resistivity of the cake are results of the simulation.

2. If the particle diameter is so small that a particle is not resolved by the computational grid, a deposited particle fills only a fraction of a voxel. Thus, many particles are deposited into a single voxel and form a porous filter cake inside this voxel. Flow can be modeled with the Stokes-Brinkman equation and parameters describing the solidity of the cake and the flow resistivity of the cake are inputs of the simulation.

Standard test dusts consist of poly-disperse particles with a wide diameter range and both cases are present: the larger particles are resolved by the grid and the smaller ones are not resolved by the grid. Thus, the filter cake forming in the simulation will consist of solid, porous and empty voxels which makes it difficult to set input parameters consistently. In particular, a partially filled voxel can only contain the smaller particles, so the local solidity and flow resistivity inside of the voxel must be different from the global solidity and resistivity of the whole filter cake.

In this presentation we will present an approach how to choose the local solidity and resistivity from resolved particle filtration simulations such that a given global solidity and flow resistivity of the filter cake is reached. This enables us to simulate cake filtration for any poly-disperse particle set at any resolution. In addition, we set a focus on the verification of the simulation results. The cake formed by partly resolved particle filtration simulations is compared to cake formed by fully resolved particle filtration simulations in terms of local solidity and flow resistivity.

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A simplified and efficient closure model for particle filtration at the porous wall of diesel particulate filters

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ABSTRACT

Due to air quality concerns, wall-flow particulate filters (better known as diesel particulate filters) are widely used for removing soot and other types of nano- and micro-particles from the exhaust gas of combustion systems. In this type of filters, gas enters in a honeycomb monolith and is forced to flow through its porous walls that act as a filter for the particles, as sketched in Figure 1.
During soot filtration, the spatial distribution of soot deposit inside the wall-flow particulate filter has a strong influence on the subsequent filter regeneration process that must be done from time to time. Therefore, a clear understanding of depth filtration and cake formation, as well as the transition between these regimes, is quite important in order to accurately determine the soot distribution along the channels of wall-flow particulate filters and hence, to predict the realistic evolution of the regeneration process [1].
Meso-scale models offer the best compromise between accuracy and computational effort [2]. In this regard, proper closure sub-model for the filtration process at the filter wall scale can significantly reduce the computational effort by reducing the number of cell devoted to the computations at the filter wall, without strongly degrading the accuracy of the overall mesoscale model.
The present study focuses on the depth filtration and cake formation occurring at the filter wall, as well as the transition between these two regimes, assuming mono-disperse particles of different sizes (from 5 nm to 1000 nm). Both 1D and lumped models are considered for the filter wall based on the homogenization approach (see Figure 2), where two different expressions for the filtration coefficient are used: the original expression obtained from unit collector filtration theory [3], and an approximated expression proposed here based on the functional fitting of the original expression. This approximated expression for the filtration coefficient is found to be very useful due to its simplicity that allows an analytical mathematical treatment of the depth filtration within the filter wall.
Model predictions are obtained with the 1D and lumped models for different variables of the filtration process, which are related with the filtration efficiency, particle deposition and pressure drop on the filter wall, during both depth filtration and cake formation. A particular attention is given to the critical time of transition between these two regimes and its simplified modeling, which to the best of authors' knowledge has never been reported in the literature for wall-flow particulate filters.
The results from the present investigation demonstrate that the lumped filtration model (with either the original or approximated expression for the filtration coefficient) yields reasonably good predictions compared to the 1D filtration model. Consequently, since the lumped model is computationally much faster that the 1D model in simulating the filtration process, it could be applied for the modeling of complete filters as a closure sub-model of the filter wall, therefore reducing the computational effort of such large simulations.

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The application of particle tracking in studying clogging dynamics in 3D porous medium

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ABSTRACT

Retaining particles from fluids to the surface of the porous medium can be used for clarification and processing of drinking water. Many factors have to be monitored regularly to maintain the performance of the filter, which could be severely changed due to clogging. Understanding the dynamics of clogging demands new techniques that could provide information about the complex interactions between fine particles and flow. Most previous experiments do not have access to the particle dynamics inside the porous medium. Part of the reason is that many porous media are opaque. In this paper, we develop the refractive index matching (RIM) method to visualize the flow field. A 3D particle tracking system has been used to follow the trajectories of the fine particles that may clog the pore throat. The dynamic information contained in their trajectories offered us a novel way to understand the particle motion in a porous medium system, which might lead us to techniques that can prevent clogging in the future.

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Revisiting Davies' Correlation for Fibrous Porous Media with Polydisperse Fibers based on Lattice Boltzmann Simulations

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ABSTRACT

Air filters are used in applications where air quality is important, notably in combustion engines (e.g. intake air filters), respirators (e.g. N95 facemask) and confined environment ventilation systems (e.g. HVAC, HEPA filters). Such porous media are usually made of fibrous materials, the composition of which will determine the efficiency of the filter to capture airborne particles as well as its air permeability. Both must be as high as possible to improve the quality factor of the filter. Two possible approaches to achieve this and resolve what may appear as conflicting requirements are the blending of fibers with different sizes and multilayering. A large body of empirical, analytical and numerical correlations have been established in the literature to predict the permeability of fibrous materials [1]. Among them, Davies' empirical correlation is the most widely used for flows at low Reynolds and low Knudsen numbers. It relates the permeability normalized by the square of the fiber diameter to a function of porosity. However, Davies' correlation, as most of the correlations from the literature, assumes a single fiber diameter and may not fully apply to polydisperse systems. Only a limited number of works have actually looked into the permeability of polydisperse and/or multilayered fibrous filters [2,3]. The one practical reason for this lies in the fact that it is virtually impossible to conduct accurate enough laboratory experiments that can clearly identify the impact of polydispersity. While some numerical investigations have attempted to define an appropriate effective fiber diameter for normalizing the permeability, they have failed in establishing a general accurate correlation. Hence, to clarify the impact of polydispersity and multilayering, more than 700 large scale simulations of flow through such porous media have been carried out using a carefully verified and validated lattice Boltzmann code. Varying systematically the composition of the filters with up to 6 different fiber sizes has allowed us to establish a modified Davies' correlation that accounts for fiber polydispersity using the coefficient of variation of the fiber size distribution and the specific surface area of the fiber blend to normalize the permeability. In this work, the numerical results are compared with experimental data from the literature and the validity of the new modified Davies' correlation is assessed. Interestingly, it is shown that the dependency of the dimensionless permeability on fiber polydispersity is weaker than what could be expected intuitively and only wide fiber size distributions are found to affect significantly permeability once normalized by the specific surface area. As a matter of fact, similar conclusions have been recently drawn for the permeability of packings of polydisperse spheres [4]. Our findings explain why it has always been difficult to experimentally quantify the impact of polydispersity. In light of these results, the impact of multilayering with various fiber sizes is also evaluated and found to be limited in absence of large fiber size ratios and/or flow inertia and slippage.

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Linking intragranular diffusion and non-equilibrium tracer transport in coarse granular drainage filters

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ABSTRACT

Diffusive mass transfer within individual grains plays a key role in the transport of dissolved compounds through coarse granular porous media, especially at high convective velocities (Passiour and Rose, 1971). The intragranular pore space contributes in fact to the immobile fraction of the total porosity, and it accounts for diffusion in response to concentration gradients between intragranular and extragranular water (Hay et al., 2011).
This work investigates the role of intragranular diffusion on solute transport, depending on granular media characteristics and flow rate. Tritium (3H2O) tracer experiments were performed at three different flux densities (0.26, 23, 41 cm h-1) and on six coarse granular hydro-physical variable drainage filters (Leca, Filtralite-P, Limestone, crushed Seashells, calcined diatomite earth (CDE), and a poorly ordered Fe oxide aggregate (CFH)) (Canga et al. 2015). Measurements of the specific surface area (SSA) following the BET method (SSABET) and the ethylene glycol monoethyl ether method (SSAEGME) indicated the presence of intragranular porosity in filters exhibiting pronounced non-equilibrium behavior.
Several fitting approaches were tested to fit the measured BTCs. The advection dispersion equation (ADE) extended with a first order removal term provided accurate prediction for approximately equilibrium transport. Non-equilibrium data were fitted by the mobile-immobile model (MIM), and revealed the presence of a large intragranular porosity. Results further showed a strong linear trend between the retardation factor (kd), responsible for non-equilibrium, and the filter materials having a large specific surface area (SSAEGME).

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Drainage filter efficiency for mitigating phosphorus losses in agricultural drainage water

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ABSTRACT

Phosphorus (P) leaching losses from agricultural land via tile drains cause eutrophication and deteriorate quality of water bodies (Ulen 2007). At present, regulatory practices appear ineffective and mitigation techniques on a long term horizon are lacking (Shoumans 2014). Targeting high risk areas and applying drainage filter technologies promise to be a cost-efficient approach to remove P from runoff (Chardon 2012). The Danish strategic research project "SUPREME-TECH" (2010-2016) (www.supremetech.dk) aims to provide the scientific basis for developing cost-effective filter technologies for treating agricultural drainage waters.
The main challenge for the drainage filters is to meet the requirements of both P sorption properties and the hydraulic efficiency at variable hydraulic and P loads. This work evaluates the hydraulic efficiency of a full scale drainage well filter composed of crushed seashells (2-4 mm) targeting P removal in agricultural drainage discharge. The porous seashell filter consists of a double-walled cylindrical wire basket (Fig 1.) allowing infiltration of drainage water from the outside to the inside of the filter. Continuous tracer tests were performed using NaCl (5 mg/l) at two different flow rates (2 and 0.1 l/s), resembling frequently occurring discharge rate of the system. Results showed a homogeneous distribution of the tracer outside the filter and the presence of a vertical concentration gradient inside the filter. Hydraulic parameters were determined by fitting the advection dispersion reaction equation (ADRE) to the measured breakthrough curves (BTCs).

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Lagrangian Models to Study Incomplete Mixing of Reactive Transport in Heterogeneous Velocity Fields

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ABSTRACT

Mixing is the process that brings reactive solutes together. Given two reactant species, their ability to react with each other is dependent on whether or not they collocate. As a result, mixing plays an important role in driving reactions. Incomplete mixing in reactive transport causes the reactant species to segregate from one another and form “islands,” therefore limiting the amount of reaction that takes place. It is important to be able to understand and describe the effects of incomplete mixing in order to accurately model reactive transport. This problem has been previously examined in purely diffusive systems, and, most recently, in a pure shear flow. The next step in addressing the issue of incomplete mixing is to explore the mixing processes in systems with more general non-uniform velocity fields, such as those describing flow through a heterogeneous porous medium. This is the problem we study here. Specifically we ask: will these types of flows enhance or attenuate incomplete mixing? And how does this impact upscaling of reaction rates? To address this question, we study reactive transport in flows through idealized heterogeneous porous media, using a Lagrangian reactive particle tracking method. In particular we aim to identify which aspects of the heterogeneous flow (e.g. shear rates, vorticity, strain rates) most control mixing and reactions, with the end goal of developing an upscaled model that incorporates these processes without the need of explicitly resolving them.

Experiments and Modeling of Microbially-mediated Calcite Precipitation in Natural Media: Build It and They Will Come

Presenter: Mohamed Nassar
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ABSTRACT

Microbially-induced calcite precipitation (MICP) was evaluated in two meter-scale “tubs” with bioaugmentation vs. biostimulation in natural unconsolidated sands. Three injection/withdrawal wells were used in each tub to facilitate strategic control of reactant injections designed to generate maximum calcite precipitation throughout the flow domain. Data collected include aqueous chemistry as well as shear wave velocities during the two-week experiment and calcite at the end of the experiment, at different locations in the tubs. Reaction extent was controlled by ureolysis kinetics which were calibrated to independent batch experiments; otherwise equilibrium conditions applied. Calcite precipitation induced changes to porosity and permeability of the system. Modeling of this coupled flow and reactive transport experiment was done by installing a multicomponent reaction network with transient flow conditions and changing medium properties into two platforms, COMSOL/iCP and PHT3D./Matlab. Both experimental and modeling results demonstrate that engineering control of the flow field coupled with (especially) biostimulation of native ureolytic organisms can induce remarkable levels of calcite precipitation leading to substantive changes in material properties.

On Pore-Scale Simulation of Reactive Flows on 3D CT images of Membranes and Rocks

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ABSTRACT

Introduction
Reactive flows in porous media are an important process in many areas of water management, including e.g. functionalized membranes for water purifications, adsorption of pollutants in soil, to name just a few. Understanding these processes and their dependence on chemical and morphological parameters poses a number of research challenges.
These processes are usually truly multiscale and developing algorithms for such problems has to be addressed. Important component of these algorithms is the pore scale simulation on images coming from 3D CT. Such simulations can be used either in solving the so called cell problems in the case of homogenization for problems with scale separation, or can be used as fine scale solvers in coupled micro- and macro- scale simulations.

Pore-Scale Simulation
Fraunhofer ITWM has developed algorithms and a software tool, PoreChem, dedicated to simulation of reactive flow on the pore-scale. It enables the investigation of the interplay between convection, diffusion, reaction rate and porous media morphology in real pore scale geometries which are either 3D CT images, or are coming from computer generated geometries. Furthermore, the code can be used in calculating the macroscopic parameters for reactive flows, based on the solution at pore scale of reactive flows. Volumetric and surface reactions can be simulated.
The flow is computed by solving the Navier-Stokes system of equations with a finite volume discretization. Transport and reactions are simulated by solving the reaction-diffusion-advection equation coupled to the surface concentration by Robin boundary conditions. For the reactions, different reaction kinetics, parametrized by reaction isotherms can be taken into account. A fast voxel based solver enables calculations directly on µCT-Images.

Results
First, a study on the effects of pore sizes and morphology on reactive transport and adsorption of pharmaceuticals in functionalized filter membranes is presented [1,2]. In the membranes, pharmaceuticals are adsorbed on functionalized surfaces, purifying the water flow in the pore space. The membrane morphology has been modeled by a parametric 3D structure model allowing variations of the geometry, starting from 3D CT image. We show the effect of the pore morphology in different regimes.
Finally, we show a study on the adsorption of MCPA in Goethite. For the study, calculations were made on µCT-Images of soil samples, containing phases with reactive and non reactive surfaces. Break through curves and concentration distributions were computed with different reaction rates.

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Upscaling Mixing and Reactive Transport in a Lagrangian Spatial Markov Framework

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ABSTRACT

First, we consider a very simple heterogeneous flow and demonstrate that the Spatial Markov model, an upscaled effective Lagrangian model that has had broad success in upscaling transport across a range of scenarios, can adequately reproduce observations of reactive transport from fully resolved models when reaction rates are heterogeneously distributed within the domain, but only when they are linear in nature. Next, we address how one might incorporate nonlinear reactions into this upscaled framework. To do so we consider recent advances in reactive particle tracking methods, which suggest that the probability of reaction between two particles can be calculated as the product of two thing (i) the probability that both particles collocate and (ii) the probability of reaction given collocation. This naturally decouples the problem as (i) depends only on transport and (ii) only on chemistry. Calculating (i) in advection-diffusion systems is relatively trivial, but here we demonstrate the challenge associated with doing so in an upscaled framework such as the Spatial Markov model and propose some ways around these challenges. In particular we demonstrate how a combined upscaling-downscaling approach can lead to reasonable estimates of mixing rates, and thus estimates of reaction rates also.

Pollutants dispersion model in the air of Mexico City

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ABSTRACT

In recent decades, urbanization and migration to cities have led to an increase in air pollution, especially in developing countries like Mexico [1] where 79% of its citizens live in urban areas and where 90% of air pollution is attributed to emissions from burning fuel in automobiles [2]. In order to generate reliable and useful information for decision makers, a comprehensive study of the phenomena involved is needed. Within a vast group of studies, the generation of pollutants dispersion mathematical models has become one of the main tools in the academic study of air quality, being a key element in most environmental impact analysis. Consequently, a 3D mass transfer model applied to the dispersion of air pollutants in the Mexico City Metropolitan Area was developed. The model was developed using the method of volume averaging [3], whereby a set of equations at the macroscopic level is generated from the scalling of equations governing the microscale. Even if the method employed is usually applied to porous media, it is applicable in the aforementioned context due to the separation of characteristic lengths, which is one of the main restraints in the methodology.
The model was developed considering a homogeneus first order reaction and Neumann boundary conditions. In order to solve the resulting model and to compute the values of the coefficent involved in it, a cell as close as possible to reality was generated by extruding polingons using the previously registered heights of the buildings present in the seltected region which has its geographical center in coordinates: 19.432845, -99.133216 and was of particular interest because: the stroke of its streets and avenues is regular; it has high concentrations of pollutants due to high traffic flow; and a large number of pedestrians are exposed every day to contaminated air. The values of the dispersion coefficient were computed by solving a closure variable problem in the described cell and a parametric analysis was carried out in order to determine the dependence of the dispersion coefficient with: the Reynolds and Péclet numbers, the Thiele modulus and with the ration between the maximum velocity and the value of the velocity in the lowest part of the system.
It was found that the geometry of the selected region plays a key role in the values of the coefficient involved in the model and the dependence of these values on dimensionless parameters was determined. It is expected that the generation of this model and the like can be used to generate relevant information for decision-making on air quality and public health.

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Formation Damage Resulting from Scale Deposition during Water Flooding

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ABSTRACT

Water flooding is the most widely used enhanced oil recovery mechanism as other methods, such as chemical methods, are based on water flooding performance. When the injected water is not compatible with the formation water, scaling and other solid deposition would occur, which reduces the formation permeability and transmissibility of the reservoir. The objective of this research is to model the in-depth reservoir formation damage as a result of scaling and to simulate its impact on reservoir performance. Scaling issue in the wellbore and flow lines has been well studied, but its in-situ deposition in the reservoir and its impact on production and recovery is still a question of interest. Thus, development of theoretical models for estimation of permeability and porosity reduction is of practical importance.

In this paper, a theoretical Carman-Kozeny based model is developed for the estimation of permeability and porosity reduction in porous media as a result of scale deposition. Additionally, the impact of affecting parameters of scaling on permeability and porosity impairment is investigated. To validate the developed model, we collected and analyzed 216 experimental data points from literature covering various thermodynamic properties and reservoir conditions. The developed model considers a wide range of factors affecting scale formation including reservoir pressure and temperature change, injection rate of the incompatible fluid, available pore volume of the medium and solubility of minerals in the solution. Moreover, statistical and graphical error analyses are employed to evaluate the accuracy and validity of the proposed model.

The results show that the proposed model is capable of predicting permeability and porosity alteration caused by scale deposition with an average relative error of 1% compared with the experimental data. Also, the values of root mean square error and coefficient of determination of the model predictions are found to be 0.024 and 0.94, respectively. Moreover, error distribution curves of the developed models show that the models do not have any significant error trend under different reservoir and thermodynamic conditions.

To study the impact of scaling deposition in the reservoir formation on the reservoir performance, numerical simulation of a synthetic field is used to simulate the production performance under a variety of scenarios. The impacts of scale deposition on pore volume reduction, permeability impairment, hydrocarbon recovery and efficiency of water flooding are investigated. Results of numerical simulation indicate that correctly modeling scaling tendency is important in capturing reservoir performance and the significance is even higher for reservoirs with low permeability.

New Insights from Imaging Pore Scale Displacements with fast X-Ray Computed Tomography

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ABSTRACT

The recovery of oil and gas involves the flow of multiple immiscible phases in porous and permeable rock. The details of this complicated multiphase flow on the pore scale is not fully understood. To a large extent that is because in the past it was not possible to directly image the flow at its natural length and time scales. Recent advances in fast X-ray computed micro-tomography have made it possible to image pore scale displacement in multiphase flow in porous rock at time intervals of 1-40 s [1,2]. By inspecting the individual radiographs from the tomography experiment, which are recorded at 40 ms time intervals, one can obtain two orders of magnitude better time resolution to study the detailed dynamics of displacements, finding characteristic decay times after individual pore scale events of 1-2 seconds [3].

The new possibilities for real-time imaging enables us to study the immiscible displacement for drainage and imbibition under dynamic flow conditions. Both in drainage and imbibition we observe that that pore scale displacement processes are non-local and cooperative, which is conceptually different than simple percolation models predict. A particularly interesting case was observed for imbibition where a complex interaction between film swelling and corner film flow ultimately leads to snap-off processes which causes the breakup of oil clusters. The large meniscus oscillations initiated by the snap-off, on the other hand, also leads to coalescence events, which again points to the cooperative dynamics in a ganglion dynamics regime. That leads to an effective transport of the non-wetting oil phase by ganglion dynamics.

The process of ganglion dynamics was studied in more detail in fractional flow experiments. The pore-scale flow regimes of connected pathway flow and ganglion dynamics have been mapped on a “phase diagram” characterized by fractional flow and capillary number which are independently chosen external parameters. An alternative representation uses a saturation - (cluster-based) capillary number parameterization which is more sensitive to the signature of ganglion dynamics. Ganglion dynamics is composed of a sequence of breakup and coalescence processes. During coalescence processes, both cluster volume and length increases, i.e. clusters move “up” a trajectory in the phase diagram. During break-up processes, on the other hand, both properties decrease and clusters move “down” the trajectory.

Ganglion dynamics occurred even though the (cluster-based) capillary number of the average flow field was at least two orders of magnitude smaller than unity, i.e. the average flow field indicates capillary-dominated regime. However viscous mobilization can also be triggered by more complex break-up and coalescence processes which have much higher local flow velocities than the average

flow field suggests. Most situations encountered are a combination of connected pathway flow and ganglion dynamics, where a combination of viscous and capillary-driven processes accounts for the net transport of oil. In imbibition we observe a co-existence of ganglion dynamics and connected pathway flow over almost the entire mobile saturation range. Static simulation approaches are not capable of capturing such regimes, as they require connected pathway flow.

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Imaging of root water uptake by MRI in combination with tracer motion

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ABSTRACT

Flow processes in natural porous media are often too slow to be monitored by direct flow imaging; therefore the visualization of such fluxes is best performed by tracer tracking. While T1 reducing contrast agents are well known in medical diagnostics, their usefulness in natural porous media is not yet well explored. As pointed out in a preceding study [1], GdDTPA is most convenient since it is very stable and does not adsorb at the soil matrix. Furthermore, it´s specific relaxivity in the liquid phase is sufficiently high to yield good contrast when used in a strongly T1 weighted pulse sequence. Here, we use a simple procedure for the quantification of tracer concentration in saturated and unsaturated natural porous media, where the reduction of relaxation times by desaturation and inhomogeneous moisture distributions are compensated for by a reference measurement. The procedure is applied to examples from natural porous media, which are decisive bottlenecks in the water flow from soil to the atmosphere: Root water uptake and evaporation from topsoil.
While plant roots take up water from the surrounding soil, GdDTPA is first enriched in the neighborhood of some roots, indicating their activity. But the tracer is also enriched in a some mm thick layer around the root, the so-called rhizosphere, which appears dark in conventional MRI sequences. Although this layer has been frequently interpreted as water depletion zone, the enrichment of GdDTPA there proves the high permeability for water and solutes.

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Hydrodynamics mediates structure during abiotic growth of a calcite precipitate barrier: a combined MRI/CT study

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ABSTRACT

Strategies for sealing the geologic environment surrounding carbon capture and storage applications are a necessary precaution against leakage potential, and calcite (CaCO3) precipitation offers a means of cementation for pore spaces and fractures that is resistant to supercritical CO2 [1]. One approach to CaCO3 deposition involves abiotic reaction of aqueous CaCl and NaCO3 [1,2], which constitutes a problem in reactive transport controlled by dispersive mixing in a porous medium. The opacity of porous media has restricted most studies to simulations, bulk measurements, and experiments in 2-D flow cells [2-4], but non-invasive MRI techniques offer a means of imaging precipitate structure and measurement of flow/dispersion in 3-D geometries [5,6]. MR studies of bacterially-induced precipitation have been reported, but we present new data on hydrodynamics and precipitate structure in the abiotic case.

Reaction of equimolar CaCl and NaCO3 solutions was carried out in a flow cell designed for use in a Bruker 300 MHz system. The modified, glass HPLC column contained borosilicate glass microspheres (180-212 μm), and reagents were injected concentrically via the bottom endcap to produce a vertical, radially symmetric flow. With constant total volumetric flow rate (395 ml/hr), the effect of varying the inner and outer flow rates was studied using a PGSE-MRI sequence in a 64×32×1 mm slice through the column center. Images revealed reduction in spin density, dispersion, and velocity from pore-clogging near the interface between the two solutions. The morphology of the precipitate barrier depends on the relative flow rates, being thinner and more clearly defined for equal inner/outer flow. Quantitative, in-situ MRI dispersion measurements were complemented with post-reaction, high-resolution X-ray CT structural images, together yielding information essential to inform hydrodynamic models of calcite cementation processes.

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An Improved Insight into Double-Displacement Mechanisms during Three-Phase Flow in Natural Porous Media

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ABSTRACT

The behavior of three-phase flow in porous media is significantly more complicated than that of two-phase flow due to involvement of pore-scale displacement physics including double and multiple displacement chains. These displacement events regulate interface arrangements to keep the existing surface forces in balance and at minimum free energy. Although numerous studies [1-3] have been conducted using micromodels and network modeling techniques to shed light on some subtleties, the displacement behavior is not well understood. Hence, we designed and performed a set of three-phase flow experiments in water-wet Berea sandstone to provide better insights into displacement events and examine their occurrence based on in-situ contact angles. To this end, we used a unique miniature core-flooding setup integrated with a high-resolution micro-CT scanner. Fluid configurations inside the pore space were imaged to quantify the contact angle distributions for different fluid pairs. We compared the contact angle distributions with those of previously performed two-phase experiments. This comparison along with pore-scale images was used to find dominant double-displacement mechanisms under three-phase flow conditions.

The experiments were performed on a miniature vertically oriented core sample using a brine/oil/nitrogen fluid system at 5.52 MPa pore pressure and 6.21 MPa overburden pressure. All three phases were equilibrated prior to the experiment. The core initially saturated with water was subjected to partial primary oil drainage followed by gas injection, a waterflood, and then an oilflood. The displacement sequences resulted in a three-phase saturation path shown in Figure 1. The core sample was scanned after each flood when no changes were observed in fluid configurations. The images were then analyzed to determine contact angle distributions for oil-water, gas-oil, and gas-water pairs under three-phase flow conditions.

Distributions and statistics of oil-water contact angles during secondary gas injection was similar to the receding one of the two-phase oil-water experiment, implying that the majority of displacements were double-drainage (i.e., gas-to-oil-to-water displacements). The observed pattern of gas-oil contact angles during waterflooding showed a bimodal distribution with an average value falling within the mean values of receding and advancing gas-oil contact angles in the two-phase experiment. This reveals that both water-to-oil-to-gas and water-to-gas-to-oil displacement events took place. Direct observation of the fluid occupancy using micro-CT images provided further evidence to support the above-mentioned findings. Interestingly, the observations showed that the oil displaced by water might invade gas-filled elements, move gas-oil interfaces toward the center of the elements, and trap the gas through snap-off. A three-dimensional visualization of a trapped gas cluster surrounded by oil is presented in Figure 2. During the oilflood, the gas-water contact angle distribution was similar neither to the receding nor to the advancing distribution of the two-phase experiments. No significant oil-to-water-to-gas or oil-to-gas-to-water displacements were observed. However, gas-water interfaces changed to maintain the free energy at minimum, a key factor governing fluid-fluid interfaces in the pore space.

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Magnetic Resonance Imaging, a tool to quantify preferential flow in complex artificial soil: a column experiment

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ABSTRACT

In soil, the presence of heterogeneous structures such as earthworm burrows, plant roots or soil cracks (also termed as macropore) may create preferential flow paths for the transport of gas, liquids and particles. Being able to assess the relative contribution of preferential flow over matrix flow is of a crucial importance for understanding different environmental problems such as the transport of contaminants in the vadose zone, the aquifer recharge or the water availability for plants. Despite its importance, the characterization of preferential flow remains a complex task. Magnetic Resonance Imaging (MRI), as a non-invasive scanning technique sensitive to volumetric water content, arises as a promising tool to analyze the dynamic of water flow in presence of preferential pathways. Though presenting a lower spatial resolution than X-ray microtomography, MRI offers the advantage to allow the optimization of the image contrast between involved phases, notably by using convenient tracers (Cuny et al. 2015). However, its use with natural soil may be hindered by the very fast relaxation of the signal that may occur in finer pores.

To circumvent this issue while assessing the usefulness of the method to detect and quantify preferential flow, we built an artificial soil sample with materials known for their relatively long relaxation time and submitted it to a tracer experiment monitored with MRI. In order to test the suitability of the method for parameter estimation, expected hydraulic properties of the materials present in the sample were compared to those estimated from MRI data.

The sample mimics, to a certain extent, some geometrical characteristics of large real macropores such as earthworms burrows. Prior to the tracer test, we first slowly saturated the sample with tap water. Then, we injected from the top a pulse of paramagnetic tracer, Gd-DTPA2-, a common medical contrast agent known to be highly conservative. The tracer concentration was adjusted to achieve the best contrast between the voxels with and without tracer following the approach proposed in Haber-Pohlmeier et al. (2010). In order to monitor the tracer transport dynamically, the sample was placed in a 1.5-T scanner and was submitted to a Fast-Spin Echo 3D sequence with short repetition time so that the whole sample was imaged with a good resolution in a relatively short time frame.

From the T1 weighted images obtained and from the evolution of voxels intensities during the experiment, we observed that the tracer effectively moved faster through interconnected macropores. We also observed some diffusion of the tracer from the macropores into the matrix. Furthermore, the hydraulic parameters of the different materials estimated with MRI data proved to be in good agreement with the ones provided by the manufacturers.

These first results show that MRI can provide high-resolution 3-D data on the time-evolution of

nonreactive solute transport in artificial soil and that MRI has the potential to be used as a quantitative tool for the characterization of preferential flow in large macropores.

Future experiments should be conducted on real soil cores with MRI sequences suited to very short signal decay.

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Utilizing fast microtomography to quantify the production and evolution of interfacial areas and curvatures of dynamic, two-phase flow experiments in a 3D porous media

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ABSTRACT

Many important subsurface mechanisms, such as geologic CO2 sequestration and groundwater remediation, involve multi-phase flow under dynamic conditions. The standard experimental technique for visualization of these mechanisms in 3D is x-ray computed microtomography (µCT), a non-destructive technique that allows for the construction of a 3D image from hundreds of 2D x-ray images acquired at different rotational angles. Until recently, a pseudo-equilibrium constraint was imposed on these µCT flow experiments to mitigate blurriness resulting from movement of interfaces during imaging. This imposition of a static flow condition poses the question of whether these experiments are truly indicative of the simulated mechanism. With the introduction of fast µCT, images can now be acquired under dynamic conditions and be used to validate and inform more comprehensive multi-phase flow theories.
One such two-phase flow theory introduces specific interfacial area to the pressure-saturation curve to try and fully describe the state of the system by eliminating the universally observed hysteric relationship between capillary pressure and saturation (Joekar-Niasar and Hassanizadeh, 2012). This theory has been researched in 2D micromodels and compared under dynamic and equilibrium conditions (Karadimitriou et al., 2014). We will present novel 3D data on the dynamic evolution of interfacial area using fast µCT. This data was acquired in a porous, glass bead column with drainage and imbibition experiments being executed under both dynamic and quasi-equilibrium conditions. Comparisons between dynamic and equilibrium states are drawn with the measurement of evolving interfacial areas, curvatures, and the trapping behavior between the two flow conditions.

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The next frontier in laboratory-based micro-CT scanning: in-situ, time-resolved imaging of dynamic processes

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ABSTRACT

Laboratory based X-ray computed micro-tomography or micro-CT has provided unique insights in the internal structure of porous materials in the past decade. Furthermore, the non-destructive nature of micro-CT scanning makes this technique ideal to monitor changes in the pore structure over time. While the spatial resolution of micro-CT systems is constantly improving, with resolution below 100 nm for some systems, the temporal resolution is still limited to several minutes or hours. This limitation is mainly due to restrictions in X-ray flux in laboratory sources, resulting in poor image quality for short acquisition times. This time restriction is often a bottleneck for imaging dynamic processes and, in general, limits the applicability to relatively slow pore scale processes occurring in the order of hours to days.

A second complication for in-situ, time-resolved imaging is the configuration of lab-based micro-CT setups. Micro-CT setups typically have the tube and detector at fixed positions and rotate the sample, as this is mechanically less complicated and more suited to obtain high-resolution scans. However, this implies that samples should be able to rotate freely without being influenced by this rotation. This is in general problematic when samples are attached to peripheral equipment, where (high pressure) flow and sensor lines limit the rotation.

To overcome these issues, the centre for X-ray tomography of the Ghent University (UGCT) and X-ray Engineering (XRE) have jointly developed a gantry-based micro-CT system of which the X-ray tube and detector rotate continuously in a horizontal plane around the fixed sample. With this system temporal resolutions in the order of seconds can be obtained[1,2]. This is possible through an efficient hardware design with a fast flat panel detector, in combination with custom X-ray transparent peripheral equipment to increase X-ray flux and dedicated 4D software tools in acquisition, reconstruction and analysis to optimize signal to noise. In this presentation the possibilities of the technique are illustrated with pore scale experiments such as the visualization of two-phase flow and solute transport (figure 1) and the methods to improve X-ray flux and optimize image quality are discussed. Furthermore, we discuss how an extensive integration of fast imaging experiments with sensor measurements (e.g. salinity and pressure) can not only help to link behavior at the pore scale to the effective properties at the core scale, but also to facilitate the experimental workflow, and even to improve image quality.

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Microfluidics and nanofluidics as windows into pore-scale processes

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ABSTRACT

Microfluidic and nanofluidic methods, developed primarily for medical applications, have much to offer the energy sector. This talk will focus primarily on my group's recent work in microfluidics and nanofluidics for subsurface energy operations: CO2, oil and gas underground. We are developing a suite of methods to (a) study pore-scale transport and reactivity, and (b) measure relevant fluid properties. I will discuss our work in pore-scale dynamics in steam assisted gravity drainage, CO2-Enhanced Oil Recovery, and CO2 sequestration. In addition, a real-rock micromodel etched in calcite crystal enables direct imaging of pore-scale processes with relevant geochemistry. In addition, a suite of microfluidics-based reservoir-relevant fluid measurements are presented including minimum miscibility pressure, diffusivity of CO2 and solvent in oil and brine, and bubble-point and dew-point measurements of gas mixtures. I will also overview our recent work on applying nanofluidics to understand transport in nanopores within hydraulically-fractured shale and tight oil reservoirs, as well as phase change measurements relevant to reservoir conditions.

Effect of internal control of fluid saturations on externally measured pressures porous media

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ABSTRACT

Applied electric fields modify the surface tension between a solid and a liquid and hence modify the wettability and contact angle on solid surfaces. Direct control over internal fluid distributions can be achieved by controlling contact angles that subsequently influence capillary pressures and drive motion of droplets across many millimeters. In this study, an Electro-Wetting on a Dielectric technique, EWOD, is used to: alter contact angles, merge and transport droplets on flat surfaces, and control the distribution of fluid phases.
Liquid droplets were supported on flat glass substrates that had been evaporated with a 50 nm thick layer of silver (i.e., ground electrode) and then spin-coated with a ~5-10 μm thick layer of PDMS, a dielectric material. A platinum wire was inserted into 10 μL droplets of 1M KCl-H2O and connected to a 50 Hz AC voltage source. Measurements were made for a range of voltages (Vrms ~0-425V). CCD cameras were used to measure changes in areal extent, perimeter, and contact angles. For Vrms=0, the contact angle on PMDS was 118o. For the range of applied voltages, the contact angle of the droplets changed by over 60o. These experiments demonstrated that contact angle can be controlled over a wide range of values.
Unsealed micro-models were used in experiments to merge and transport drops. In the merging experiments, three 50 nm thick electrodes were formed on the top plate separated by a gap of 0.69 mm, while the bottom plate contained a single large area silver electrode 50 nm thick. A 10 μL 1M KCl-H2O droplet was placed on the left electrode and another on the right electrode and merged when 424 V was applied to the middle electrode. The contact angle of the drops on the middle electrode decreased by 60 o relative to the portions of the drops on left and right electrodes. The resulting pressure difference translated and merged the two drops over a distance of ~1mm in ~13 seconds. These experiments demonstrate that EWOD techniques can be used to alter contact areas and interfacial area as well as merge and transport fluids without the need for an external pressure source. These results are of key importance to determine the effect of internal control of fluid saturations on externally measured pressures porous media.

Lagrangian flow investigation in three-dimensional porous medium flow

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ABSTRACT

Micro and millimodels represent a family of experimental tools allowing to investigate a whole range of problems in porous media, e.g. multiphase flows (Datta, Chiang et al. 2013) to mixing and reactions in saturated (Anna, Jimenez-Martinez et al. 2013) and unsaturated porous media (Jiménez-Martínez, Anna et al. 2015). The extensive use of these technologies is explained by the data visualization effectuated at the pore scale, as a knowledge of pore scale dynamics is key to a better understanding of these processes and also provides data sets useful for comparisons with numerical models.
Here we present some work combining three-dimensional particle tracking velocimetry (3D-PTV) to investigate flow in a Lagrangian framework, using the technique presented by Holzner, Morales et al. (2015) with X-Ray microtomography measurements of the porous medium. The registration of the 3D-PTV and X-Ray data, an operation allowing to transform both data sets in only one coordinate system, provides very useful information in order better understand the relation between flow intermittency, the structure of the porous medium and related processes like anomalous dispersion, bacterial adhesion and bioclogging or dynamics of re-mobilization of colloids.

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Oxygen Gas Bubble Growth in PEM Electrolyzers using PTL-on-a-Chip

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ABSTRACT

The proton exchange membrane (PEM) electrolyzer is a layered electrochemical device that converts water into hydrogen and oxygen gases. The PEM electrolyzer is capable of operating at high current densities and generating highly pure hydrogen gas, which makes it a promising candidate for grid-level storage systems. One of the main challenges hindering further adoption of the technology is the oxygen gas accumulation in the porous transport layer (PTL) of the anode, which leads to mass transport limitations and decreased efficiencies.

At the anode, oxygen gas is a by-product that must be removed from the catalyst layer in order to reduce mass transport losses during cell operation. The PTL is positioned between the catalyst layer and the exhaust channels, and is one of the main components in a PEM electrolyzer responsible for distributing liquid water, while simultaneously providing pathways for oxygen removal. The complex fluid interactions inside the PTL need to be better understood so that new materials can be designed for enhanced mass transport. However, there is a scarcity of in-situ visualization studies in the literature that capture the flow phenomena within the microscale pores.

In this work, the effect of the PTL structural properties on the growth of oxygen gas bubbles was investigated using a microfluidic approach, whereby gas is injected into a PTL-on-chip device. To observe realistic behaviors, the PTL-on-chip was designed to represent important structural properties of the PTL, and each experimental variable was carefully considered using dimensionless numbers, such as the capillary number. An invasion percolation algorithm [1] was employed to compare modelling results to experimental results (Fig. 1). The results showed that the oxygen gas movement is closely related to the structure of the PTL. Due to the inherent heterogeneity of the structure, different flow regimes and breakthrough behaviors were observed for different gas injection sites. The results provided insights to designing new PTLs that are capable of guiding more unidirectional gas flows to more directly remove the product oxygen gas.

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Colloid Transport In A Microfluidic Soil Analog: Population Dynamics And Single Particle Trajectories

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ABSTRACT

Low solubility contaminants such as heavy metals and radionuclides can adsorb onto mobile colloids and travel with underground water in soils over kilometers. However, the detailed flow pathway and rate-limiting transport mechanism of colloids in soils are largely unknown. To study these phenomena we developed a microfluidic soil analog to measure both population dynamics and single particle trajectories of model colloids. The soil analog consists of an O(1 mm2) chamber filled with packed 15 μm polystyrene beads. Comparisons between measured and estimated hydraulic permeability from Lattice Boltzmann Method (LBM) simulations suggest a pseudo-two dimensional packing with ~50% of beads displaced from the bottom of the channel. A T-junction at the exit of soil analog allowed for encapsulation and enumeration of several thousand colloids per experiment to give population dynamics. Single particle trajectories of 0.5, 1, and 3 μm colloids were captured by fluorescence microscopy within the soil analog at Peclet numbers of 1600-9600. Tortuosity calculated from these trajectories and comparison with LBM simulations using point particles revealed that pore-scale transport of colloids was influenced by the size exclusion effect. The innovative features of this device provide a means to link microscale transport properties like particle trajectories, which are difficult to measure in natural soils, to macroscale transport properties like dispersion, which can be measured in column and field-scale experiments. This device will enable future studies to connect micro- and macroscale colloid transport and to measure the effect of chemical heterogeneities that mimics those found in natural soils.

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Instability in micromodel porous media two phase flow due to inter facial drag

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ABSTRACT

Two phase flow in porous media is governed by heterogeneity, connectivity, wetability, fluid velocity and viscosity. We use surfactant to reduce the inter facial tension between the phases leading also to shear thinning, changing domain wetability and even create elastic turbulence. In this study we perform 2d and 3d porous media two phase flow experiments with suspended florescence beads in both phases. This allows us to quantify the inter facial influence and the dynamic it exhibits with the porous media. We show that the trapped oil ganglia experiences enhance drag from the water phase which leads to study shear and extraction of oil. By itself this process is negligible but it leads to destabilization of the capillary pressure and in turn to finger penetration. Here, we quantify this instability for various pore throats, velocity and surfactant concentration showing the relation between pore throats to the rate of finger advancement.

Smart microgels for improved flood conformance

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ABSTRACT

We designed and fabricated the microgels that can remain un-swollen in an aqueous environment for a tunable period of time from months to years. This is implemented by a core-shell structure with a hydrogel core and a degradable polymeric shell. The delayed swelling makes the microgels a promising candidate to be used in the gel treatment of reservoirs; compared to the preformed gels used currently, our new microgels with delayed swelling are more suitable for controlling the flood conformance in the deep formation. We demonstrate the concept by flowing the microgels into a stratified 3D micromodel with two distinct permeability and directly visualizing the microgels and two liquid phases using confocal microscopy. The micromodel experiment confirms that the microgels effectively block the pores in the high-permeability stratum. The displacing fluid then takes the originally low-permeability stratum and reduces the residual oil there. the quantified study regarding the effects of microgel concentration, stiffness, and flooding volume is ongoing.

Effect of permeability on local velocity distribution in 3D porous micromodel

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ABSTRACT

We study the dynamics of single phase fluids in a 3D model porous medium with variable pore sizes. The micromodel is a packing of sintered beads in a quartz capillary. The pore sizes are varied by mixing two different bead sizes at different ratios. Using confocal microscopy we are able to visualize the fluid velocities within the porous media [1]. We measure the bulk permeability of the medium using Darcy's law simultaneously. The medium permeability strongly depends on the pore sizes and decreases for smaller pores. We show that the velocities have exponential probability distributions for all different pore sizes [2]. However, when normalized by Darcy velocity the exponents vary considerably. We propose a scaling for velocity distribution that depends on the directly measured permeability. At constant flow rate the average velocity scales with inverse square root of permeability.

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Measurement of the Lagrangian coherent structure in porous micromodel

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ABSTRACT

We measure the Lagrangian coherent structure and mixing in a 2D model porous medium. The 2D micromodel is made with soft lithography and is based on a slice of 3D porous micromodel. Using confocal microscopy we are able to visualize the fluid velocities within the porous media [1]. Using PIV technique we are able to fully characterize the steady state flow within the micromodel. The flow velocities have an exponential distribution with a large population close to the average value. We investigate how the disordered porous media modify the fluid stretching of the fluid within the medium. By measuring the Lagrangian coherent structure in the medium, we find that the fluid experiences the largest stretching close to the beads. The distribution of stretching in the medium has an exponential decay indicating that in most locations in the medium there is an average small stretching while in rare locations there are much larger stretching. The measurement of the stretching is a metric to identify the divergence of concentration of material in the medium [2].

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Effects of pore size and geometry on polymer flooding efficiency in microfluidic pore networks

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ABSTRACT

"The effect of pore size and geometry on polymer flood efficiency in porous media: an experimental study."

The efficiency of enhanced oil recovery is strongly dependent on the pore structure and geometry of porous media, influencing the competition among various forces defining the patterns and general dynamics of multiphase flow in porous media. Other important factors affecting oil displacement are the properties of the fluids that define the patterns and general dynamics of multiphase flow. This motivated many studies to evaluate the efficiency of various injecting fluids such as foam, polymer solutions, and water on oil displacement and general dynamics of two-phase flow in porous media [1-4]. In the present work, we have conducted a comprehensive series of microfluidic experiments to delineate the effects of pore size distributions and shape on the efficiency of polymer flooding in porous media saturated by oil. The impact of pore structure and geometry on To do so, we have conducted micro-fluidic experiments using micromodels. The micromodels have been fabricated based on X-Ray computed tomography images of a sand-pack with varying grain sizes leading to a more realistic pore network representation of a reservoir pore network. The micromodels were fabricated in a silicon wafer using standard photolithography and inductively coupled plasma–deep reactive ion etching methods. Three micro-models with well-defined pore size distribution were fabricated and used in our experiments. The micromodels were initially saturated by Silicone oil. The displacing fluids were aqueous solutions with dissolved xanthan gum whose rheological characteristics were accurately determined by a stress controlled rheometer. The dynamics and patterns of the interface displacement as well as the size distribution of the trapped oil ganglia were visualised using an optical microscope. Over one hundred experiments were conducted to evaluate the effects of several parameters such as injection rate, polymer concentration (affecting fluid properties), and pore size distribution and shapes of porous media on shear-thinning fluid flow with well-defined rheological properties and oil displacement efficiency. In addition, our analysis extends the understanding of the mechanisms influencing phase entrapment and general dynamics of immiscible-two phase flow in porous media in the presence of shear-thinning fluids.flow is not well understood. This work aims to use micromodel experiments conducted on a realistic pore network to better understand the effect of pore geometry on flow. The relationship between pore shape and flow will be examined using digital image analysis to make both quantitative and qualitative assessments.
In this work a number of experiments have been carried out using 3 silicon micromodels with varying pore sizes and geometries. The micromodels have been fabricated based on X-Ray computed

tomography images of a sand-pack with varying grain sizes leading to a realistic representation of a reservoir pore network. In the experiments, varying polymer concentrations have been used to displace oil at a number of different flow rates. The results from these experiments have then been compared with digital image analysis of the porous media used in the different experiments to draw conclusions on the relationships between pore shape and size characterisations and their effects on flow.

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Velocity structures in 2D porous micromodels: a micro-PIV study

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ABSTRACT

Single- and multi-phase flow in porous media is pervasive in natural and engineering systems with applications such as geologic CO2 sequestration, enhanced oil recovery, and ground water remediation. A key objective of research in this area, is improving the accuracy of numerical models used for field-scale simulations by incorporation/better representation of the pore-scale flow physics. This necessitates experimental data for developing, testing and validating such models. We have studied single- and multi-phase flow processes in two-dimensional porous micromodels with different geometries at different flow conditions. The microscopic particle image velocimetry (micro-PIV) technique is used to obtain spatially- and temporally resolved velocity vector fields. The flow statistics are used to extract key flow features and their relation to the geometry of the micromodel.

Measurement of flow diversion and velocity fluctuations due to polymer retention in 3D micromodel of porous media

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ABSTRACT

We use confocal microscopy and bulk permeability measurements to probe the effects of polymer flow on the permeability and microscopic velocity distribution of a single phase flow in 3D micromodel of porous media [1]. The medium permeability decreases after polymer flow [2], while the average microscopic flow velocity in the medium increases. The local changes in fluid velocity after polymer flow are inhomogeneous, with the flow in some pores being diverted, while other pores experience a faster flow. The distribution of velocities normalized by the interstitial fluid velocity has a wider distribution after polymer flow, further indicating greater flow heterogeneities as polymer is retained within the medium[3]. We also show that at constant volumetric flow rate the magnitude of fluid velocities scales with the inverse permeability, collapsing the velocity distributions onto a single curve.

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A Streamline-based Approach for Evaluation of Electrical Tortuosity of Porous Media Using Electrical Conductivity

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ABSTRACT

Quantifying pore network structure and taking that into account in interpretation of borehole geophysical measurements is a must for reliable assessment of permeability and fluid saturations. Conventional methods for interpretation of electrical conductivity logs usually assimilate pore network characteristics such as tortuosity through calibration efforts. There have been previously developed random-walk algorithms, which calculate the tortuosity of the pore network from the mean-square displacement of the random walkers. Nevertheless, it doesn't provide a way of visualizing how the internal heterogeneity of the rock structure affects the tortuosity. Streamline-based simulation of electric currents is an attractive alternative because it allows the estimation of tortuosity, provides different forms of visualization, and it could be potentially faster compared to random-walk algorithms since it does not require statistical averaging. Furthermore, it provides the possibility of using borehole electrical conductivity measurements for assessment of pore network structure.

The objectives of this paper include (a) developing an algorithm to quantify the rock's directional tortuosity based on the spatial distribution of the electrical current's streamlines, (b) applying the concept of time-of-flight to electrical charges and use it to improve the tortuosity assessment, (c) providing a visualization tool of the tortuosity and its anisotropy, and (d) comparing the results obtained from the streamlines with the ones obtained from the random-walk method when applied to the same rock samples.

In order to accomplish the aforementioned objectives, the first step is to obtain the three-dimensional rock pore-scale images using a Micro-CT scanner. Electrical conductivities are assigned to each voxel according to their content (e.g., water, oil, clay, and non-clay minerals). An arbitrary potential difference is applied between two opposing surfaces of the rock image, and the remaining external boundary conditions can be chosen as either no-flux (non-conductive walls) or periodic. The electrical potential distribution is then calculated from the solution of the Laplace equation. Next, the streamlines and their respective time-of-flights are calculated from the electrical flux distribution and they are used to estimate directional tortuosity of the rock samples.

We successfully applied the developed simulator to synthetic and actual rock samples taken from carbonate formations with complex pore geometry. The simulator was initially validated with synthetic cases for which analytical calculations could be performed and the results were exact up to the numerical precision of the computer. The results obtained from the actual rocks were also coherent in comparison with the ones obtained by using the random-walk method. Even though streamlines have been used before to evaluate the tortuosity of porous rocks, the concept of time-of-flight has not been applied to electrical currents before. The application of this method improves the assessment of electrical tortuosity from well logs, which also leads to a better assessment of the directional connectivity. Since previous studies have shown that there is a persistent correlation between the directional connectivity and the formation factor at different scales, the streamline-based electrical

tortuosity approach can also improve the correlation between petrophysical properties from core scale to log scale.

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Power exponential velocity distributions in disordered porous media

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ABSTRACT

Velocity distribution function (vdf) link the micro- and macro-level theories of fluid flow through porous media. Several reports, by different research groups, about vdf in porous media are already available. The findings, however, appear to be inconsistent with each other. On the one hand, theoretical [1], experimental [1] and numerical [2] results suggest that the vdf can be approximated by a Gaussian. On the other hand exponential [3, 4] or even stretched exponential [5] functions were also reported.

To reconcile these contradictions, we propose that the velocity distribution functions follow the power exponential distribution. Using the Lattice Boltzmann Method we verify our hypothesis in a stochastically generated porous media. To this end we study distributions of the fluid absolute velocity and its longitudinal and lateral components relative to the macroscopic flow direction in various configurations, porosities and boundary conditions.

We claim that all these velocity distributions follow the power exponential law controlled by an exponent and a shift parameter and find how these parameters depend on the porosity [6].

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On the limitations of one- and two-temperature models for natural convection in porous media

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ABSTRACT

A direct-numerical-simulation is employed on a 2-dimensional Horton-Rogers-Lapwood convection problem in a regular porous medium. High resolution direct numerical simulation has been performed by means of the thermal lattice-Boltzmann method (LBM). The governing equations are solved at the pore-scale level in both the fluid and solid phases while conserving the appropriate conjugate boundary condition at the solid-fluid interface. This allows us to calculate continuum-scale parameters such as the permeability and the stagnant thermal conductivity of the medium very accurately without using any empirical formulations. Also, the regular arrangement of the solid blocks allows us to calculate the intrinsic-averaged temperatures of each phase in the porous medium. This information is used to test the validity of one- and two-temperature models in predicting the thermal behavior of the system for a range of Rayleigh numbers. We perform the simulations for different values of solid-to-fluid thermal conductivity ratio and the pore-scale results are compared with corresponding theoretical and experimental data.
The comparison shows that the classical continuum Darcy- local thermal equilibrium models are only valid when solid and fluid phases have similar thermal conductivities. However, for a porous medium with highly conductive solid matrix, e.g. in steel-water configuration, the pore-scale results predict significantly lower Nusselt number than continuum Darcy- local thermal equilibrium models; while the pore-scale results are consistent with the experimental data. On the other hand, when the fluid phase is more conductive than the solid matrix, the pore-scale results predict higher values of Nusselt number compared with the classical continuum Darcy- local thermal equilibrium models. The detailed temperature fields from the pore-scale simulation also show that the observed deviation cannot be linked to the lack of thermal equilibrium between the solid and fluid phases. Detailed discussion is then made to link the observed thermal behavior to a new form of thermal dispersion phenomena that cannot be explained by the currently available thermal dispersion models for convection in porous media. Finally, a new upscaled energy model is proposed which incorporates the observed thermal features which cannot be explained and predicted by the commonly used one- and two-temperature models.

A Hierarchy of Thermodynamically Constrained Averaging Theory Models for Two-Fluid-Phase Flow in Porous Medium Systems

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ABSTRACT

It is widely understood that the traditional model for two-fluid-phase flow in porous medium systems does not represent explicitly important pore-scale physics, relies upon inaccurate assumptions about the dependence of fluid pressures and saturations, and must be closed with hysteretic relationships. The thermodynamically constrained averaging theory (TCAT) is an approach for directly linking the pore-scale with the macroscale. In this work, we illustrate components of the theory, and derive a hierarchy of models of varying sophistication. This hierarchy is shown to reduce to the traditional model under a restrictive, and unrealistic, set of assumptions. Other models from the hierarchy are formulated and the novel components of the TCAT models are summarized, which include kinematic evolution equations for entity extents, and a dynamic interfacial area relaxation mechanism. The novel components of the model are shown to require new macroscale closure relations for kinematic velocities; a relationship among interfacial curvatures, fluid saturations, and interfacial areas; resistance tensors; and for the more advanced models common curve properties and contact angles. Because of the firm connection across scales, microscale experimental observations and modeling can be used to evaluate mechanism included in the TCAT model and provide the elements needed for model closure and validation. We briefly summarize a rapidly growing body of available work validating this new class of model.

Analyzing Two-Fluid-Phase Flow Dynamics Using Micro-models

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ABSTRACT

Microfluidic approaches provide an opportunity to observe phase distributions, interfaces, and common curves at high spatial and temporal resolutions in two-fluid-phase porous medium systems. Such observations provide an opportunity to visualize mechanisms, determine closure relations needed for existing and evolving models, and provide a means to validate theoretical predictions. We use a 500-micron cell with a circular solid phase to study two-fluid-phase displacement, including a dense pattern of drainage, imbibition, and scanning curves at very high spatial and temporal distribution. A lattice Boltzmann method (LBM) is used to model the experimental data and shows excellent agreement for equilibrium states and certain aspects of the dynamics. Pressure dynamics, displacement processes, and interface curvature change time scales are shown. Further, the fluid pressure, saturation, curvature, and interfacial area data is compared to mechanistic predictions based upon the thermodynamically constrained averaging theory (TCAT), validating key aspects of the theory.

Dynamic permeabilty – Experimental investigations and numerical analysis

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ABSTRACT

Transient permeability tests, i.e. pressure diffusion and/or pore pressure oscillation methods, allow to measure the intrinsic permeability and the storage capacity of tight rocks in reasonable time with good signal-to-noise ratio, [2]. In such time-dependent or harmonic permeability tests, only pressure transients have to be measured experimentally in the upstream and the downstream reservoir. Subsequently, pressure amplitude differences and phase shifts can be determined. Finally, in a post-processing step, storage capacity and effective permeability can be determined from the solution of a pressure-diffusion equation, [1]. Further, inertia effects can be taken into account allowing to introduce a “dynamic” permeability coefficient.

In the present contribution, we discuss advanced experimental setups for harmonic permeability tests. Basically, the setup consists of a magnetic shaker which is coupled through a rubber membrane with the upstream reservoir. High-sensitive dynamic piezoelectric sensors allow for measuring the pressure transients in the up- and downstream reservoirs. In addition, it will be discussed, how the data analysis in the post-processing step could be improved by reformulating the pressure-diffusion equations in form of (complex) Helmholtz equations.

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Time-lapsed monitoring of thermo-mechanical loaded porous rock to identify relations of rock fracture behavior and effective thermal conductivity

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ABSTRACT

Experimental and theoretical study of the wave propagating through homogeneous medium has been analysed by several researchers in the past decades including, Viggiani and Atkinson 1995, Jun-Ung et.al. 2008, Wuttke et.al.2012, Dai et.al. 2013. Although the phenomenon of wave propagation through the heterogeneous and dispersed medium is complex, the complexity is further increasing if the medium changes its solid or fluid phase properties during the process of evolution. From the past studies, it is explicitly clear that the wave field carries an important information of the medium passing through it. The monitoring of transient changes in porous structures plays an important role for parameter identification, process monitoring and micro to macro parameter detection in geoscience and geotechnics.

In the presented study, the Coda wave interferometry (CWI) is used to identify the smooth and time-lapsed macroscopic change during the penetration of a bentonite slurry front into fluid saturated coarse geomaterial. The study provides the important information on the penetrating bentonite front shield into coarse-grained material during the tunnel drilling process and the resulting stability of the tunnel front shield. The quest during this process results in the understanding of the changes of the effective macroscopic shear parameter of the multi-phase porous geomaterial. This paper show the principle application of the CWI method on lab experiments and its ability as a monitoring method of transient processes in porous geomaterials.

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Transient vs steady-state techniques for determining effective thermal properties of porous media

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ABSTRACT

Accurate determination of thermal conductivity and/or diffusivity of porous media or soils in particular is vital in performing analysis and modeling operations in a range of fields of engineering, agriculture, hydrology, and others. In engineering applications, thermal conductivity plays a significant role in the operation of small and/or large scale ground heat energy storage, embedding of underground power cables in selected porous media, nuclear waste disposal facilities, heat exchanger piles of structures, assessing the effect of berms on the heat loss from thermal energy storage tanks, etc. Depending on the type, thermal properties and medium temperature, transient or steady-state techniques are employed to obtain the thermal conductivity or diffusivity of porous media.

In this paper, the thermal conductivity of three fine-grained soils of low plasticity (termed here as soils A, B and C) analysed using transient and steady-state techniques is presented. The transient thermal conductivity of the soils was measured under room temperature and atmospheric pressure conditions with a Decagon KD2 Pro TR-1 thermal needle probe, based on transient line source measurement in compliance to ASTM D5334-08 (2008) and IEEE 442 standards (1992), Figure 1 (left). The sufficient length (100 mm) to diameter (2.4 mm) ratio of the probe ensures that conditions for an infinitely long and infinitely thin heating source are met. In Figure 1 (right), the experimental results are compared with prediction of Johansen (1975) and Lu et al. (2007) models.

Figure 1. Transient needle probe set-up (left) and variation of transient thermal conductivity with volumetric water content (right)

The steady-state thermal conductivity of the investigated soils was obtained at specific hydro-mechanical conditions using a steady-state thermal conductivity meter, Sass and Stegner (2012). The apparatus consists of a top heating plate, a bottom cooling plate and a reference disc with known thermal conductivity, Figure 2 (left). The specimen is sandwiched between the top heating and reference plates. The temperature distribution within the soil sample and reference disc obtained using COMSOL Multiphysics is shown in Figure 2 (right). The measured values of reference disc temperature T2 required for obtaining the steady-state thermal conductivity of the soils are plotted in Figure 3.

Figure 2. Steady-state thermal conductivity measurement set-up (left) FE mesh (middle) and temperature distribution in sample and reference disc (right)

Figure 3. Observed values of reference disc temperature T2 for the three fine-grained soils

The transient thermal conductivity of the three soils ranged from 0.173 W m-1 K-1 to 0.215 W m-1

K-1 in dry condtion, and from 1.303 W m-1 K-1 to 1.574 W m-1 K-1 in saturated condition, respectively. For the steady-state measurements, the thermal conductivity ranged from 0.240 W m-1 K-1 to 0.248 W m-1 K-1 in dry condtion, and from 1.248 W m-1 K-1 to 1.259 W m-1 K-1 in saturated condition, respectively. The measured transient thermal conductivity of the soils showed higher dispersion as compared to the steady-state measurements. Overall, the transient technique provided lower thermal conductivity in dry condition, and higher values in saturated condition, respectively, as compared to the steady-state technique.

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Permeability anisotropy tests and a biphasic material model for undisturbed peat

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ABSTRACT

Peat deposit consists of partially decomposed vegetation remnants accumulated in water-logged conditions. The high water content, extreme compressibility, structural anisotropy and the likely compressible organic solid particles propel peat as a geotechnically challenging material in both laboratory testing and numerical modelling. In this study, the cross-anisotropic permeability of an undisturbed Irish peat was studied in falling head permeability tests and was compared with the coefficient of permeability calculated indirectly from one-dimensional oedometer consolidation tests. Both of the results demonstrated that the coefficient of permeability of vertical specimens (horizontal fibre alignment) was marginally larger than that of the horizontal undisturbed peat specimens at their undisturbed state. The similar values of the vertical and horizontal permeabilities on the undisturbed peat indicated that occurrence of fibres did not introduce permeability anisotropy at the initial conditions. The coefficient of permeability decreased one order of magnitude with a void ratio change from 11 to 7. A solid hyperviscoelastoplastic model within the thermodynamically consistent framework was extended by using the effective stress concept to model the biphasic mechanical properties of the undisturbed peat subjected to the one-dimensional oedometer consolidation tests. The constitutive model was proposed for the finite-strain, macroscopic responses of the porous hyperviscoelastoplastic solid and the pore water, where both of the constituents were assumed to be incompressible. The coefficient of permeability was formulated in a power law of the volume fraction change based on the experimental results. The model was implemented as UMAT in the Finite Element software ABAQUS. For small strain condition, the model was verified against Terzaghi's theory of one-dimensional consolidation [1]. The simulation results on the large strain consolidation behaviour of peat showed fair agreement with the experimental data.

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Pressure Dynamic Analusis of Shale Gas Reservoir Based on Boundary Element Method

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ABSTRACT

At present, conventional analytical method used in the shale gas reservoir pressure dynamic analysis is too difficult to be solved. In addition, the method of numerical calculation is too slow.So the semi-analytical method for shale gas reservoir pressure dynamic analysis receives great attention.This paper adopts boundary element method to analze shale gas reservoir pressure dynamic characteristics with consideration of shale gas desorption, diffusion migration mechanism.In this paper,boundary element method(BEM) is established on the basis of single and compressible fluid flowing mathematical model by Laplace alteration. And BEM changes governing differential equations to integral equations of boundaries.Several pressure behaviors are analyzed by associating with curve charts worked out with this method.It offers technical support for shale gas reservoir parameters,deliverability evaluation and more flexible theory method for well test analysis.

Multiphasic modelling of human brain tissue for tumour-treatment applications

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ABSTRACT

A surgical intervention is often required if the functionality of the sensitive human brain tissue is seriously compromised, as for example in case of malignant brain tumours. A promising method for an effective treatment of these tumours is provided by the so-called convection-enhanced drug delivery (CED) [1]. Therein, a direct extra-vascular infusion of a therapeutic solution is applied via catheters within the brain-tissue. By this means, the aim of this contribution is to simulate the expected effects as well as coupled impacts of a scheduled surgical procedure with numerical computations based on a sophisticated multicomponent and multi-physical theoretical modelling strategy applied to the human brain tissue.

The enormous microscopical complexity of the multicomponent brain-tissue motivates the application of the well-known Theory of Porous Media (TPM), which is based on a volumetric homogenisation of the underlying microstructure of solid and fluid components over representative elementary volumes (REV). This procedure leads to an idealised macroscopical model of superimposed and mutually interacting constituents. In the present case, the model proceeds from immiscible and miscible fluid components, thus inducing a quaternary model [2] for the description of the drug-delivery problem within the brain tissue. In particular, the model is based on an anisotropically deformable solid skeleton, provided by tissue cells and vascular walls, which is perfused by two mobile liquids, the blood and the interstitial fluid. Furthermore, the latter is treated as a real mixture of two components, the liquid solvent and the dissolved therapeutic solute. In addition, the anisotropic permeability of the brain tissue is considered by a spatial diversification of the coefficients of the permeability tensor obtained from diffusion-weighted Magnetic-Resonance Imaging (DTI).

For the numerical solution of the arising coupled partial differential equations, the system is discretised in space by the Finite-Element (FE) Method and in time by an implicit (Euler) time-integration scheme, which is then monolithically solved by use the in-house FE solver PANDAS. Numerical examples demonstrate the applicability of the presented model for selected problems. In particular, the anisotropic therapeutic spreading of the infused drug, using a single catheter or multiple infusion catheters, and accompanying coupled effects (such as local deformation or pressure states) are shown.

However, the straight-forward monolithic solution yields immense numerical costs. Therefore, suitable model-reduction techniques, such as the method of proper orthogonal decomposition (POD) [3, 4] splitting the overall problem in offline and online computations or the discrete-empirical-interpolation method (DEIM), are applied to reduce the online computation time significantly while maintaining the detailed theoretical basis of the modelling approach.

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Microscale hydrogel particles as templates for porous, composite tissue scaffolds

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ABSTRACT

Synthetic and natural hydrogels have found widespread utility as cell carriers for tissue engineering scaffolds and surrogate extracellular matrices for fundamental and clinical biomedical applications. Hydrogel properties arise from macromolecular architecture and persist across many length scales, from nano- to macro-scales. While synthetic hydrogel-forming macromolecules, such as polyethylene glycol diacrylate (PEG-DA), are extremely fungible, scaling mechanical, diffusive, and biofunctional properties across six orders of magnitude in length is a daunting challenge. To bridge molecular and macroscopic scales, we have developed a “lost wax” fabrication technique that produces highly-porous hydrogels via the assembly of photolabile hydrogel microsphere networks, which are subsequently encapsulated and sacrificed to create macroporous hydrogels. This approach relies on two enabling innovations: 1) a microfluidic device that enables the continuous and high-volume production of monodisperse photopolymerized PEG-DA hydrogel microspheres synthesized in absence of dissolved oxygen; and 2) microfluidic flow-assisted self assembly of particle structures and their optical manipulation. First, multifunctional photodegradable PEGDA hydrogel microparticles were prepared by microfluidic emulsification, oxygen purging and in situ photopolymerization. These particles were next assembled via microfluidic patterning to create hydrogel colloidal crystals (CCs) and inverse colloidal crystals (ICCs). Both CCs and ICCs have found widespread application use in a variety of fields including photonics, catalysis, and more recently cell-motility platforms due to their high surface area, regular orientation and remarkable optical properties. Traditionally, however, the fabrication of ICCs, are limited to materials that can withstand harsh processing conditions such as organic solvents or high temperatures. Here, however, we exploit photolabile PEG to polymerize microscale biocompatible, multifunctional PEG-DA ICCs directly within microfluidic devices.

Porous Membrane for Microfludic Device

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ABSTRACT

Microfluidic devices and channels allow for the creation of in vitro models such as lung-on-chip to study biological barriers that would otherwise be difficult or impossible. In this work, we will fabricate membranes in the microfluidic device and study the effect of porosity on the transport of drugs and nanoparticles through the membranes.

Dispersion of Geometric TiO2 Nanomaterials and Their Toxicity to RPMI 2650 Cells

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ABSTRACT

Titanium dioxide (TiO2) based nanofilaments—nanotube, nanowire, nanorod—have gained interest for industrial, electrical, and as of recent, medical applications due to their superior performance over TiO2 nanoparticles. Safety assessment of these nanomaterials is critical to protect workers, patients, and bystanders as these technologies become widely implemented. Additionally, TiO2 based nanofilaments can easily be inhaled by humans and their high aspect ratio, much like asbestos fibers, may make them
toxic in the respiratory system. The tendency of TiO2 nanofilaments to aggregate makes evaluating their nanotoxicity difficult and the results controversial, because incomplete dispersion results in larger particle
sizes that are no longer in the nano dimensional size range. TiO2 nanofilaments are aggregated and difficult to disperse homogeneously in solution by conventional methods, such as sonication and vortexing. In this study, a microfluidic device was utilized to produce stable, homogeneous dosing solutions necessary for in vitro toxicity evaluation by eliminating any toxicity caused by aggregated TiO2 nanomaterials. The toxicity results could then be directly correlated to the TiO2 nanostructure itself. The biocompatibility of four TiO2 nanogeometries—nanotube, nanowire, nanorod, and nanoparticle—were assessed in RPMI 2650 human nasal epithelial cells. All TiO2 based nanomaterials dispersed by the microfluidic method were nontoxic to RPMI 2650 cells at the concentrations tested. Whereas 100 ?g/ml
concentrations of nanowires and nanotubes dispersed by sonication reduced viability up to 27%, indicating that in vitro toxicity results may be controlled by the dispersion of dosing solutions.

3D Printing of Viscoelastic Interpenetrating Network Hydrogels

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ABSTRACT

Interpenetrating network (IPN) hydrogel materials are of great interest as porous materials due to their unique toughness properties. In this study, an alginate-polyacrylamide IPN hydrogel formula was optimized for 3D printing using a dual syringe system where the components that initiate polymerization of each network remain separated until printing. The dual syringe system uses a single motor and mixing head to extrude both parts of the hydrogel formulation for controlled polymerization of the material. The elastic modulus, stress relaxation, shape fidelity, opacity, and print speed were quantified for the printed materials. The elastic and time-dependent viscoelastic properties (stress relaxation) were tuned to match mammalian tissues by changing the crosslink density and monomer concentration. Further, because the water swelling behavior of the printed alginate-polyacrylamide IPN was undesirable, more hydrophobic network components were examined, markedly reducing the water uptake of the hydrogels. Since the mechanical properties of this material can be tuned to mimic the elastic and viscoelastic properties of biological materials, this material may find application in a variety of biomedical applications.

Multiphoton fabrication of biocompatible collagen structures with controlled porosity

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ABSTRACT

Multiphoton fabrication is a powerful technique for three-dimensional (3D) printing of structures at the microscale. Many polymers and proteins have been successfully structured and patterned using this method. Type I collagen comprises a large part of the extracellular matrix for most tissue types and is a widely used cellular scaffold material for tissue engineering. Current methods for creating collagen tissue scaffolds do not allow control of local geometry on a cellular scale. This means the environment experienced by cells may be made up of the native material but unrelated to native cellular-scale structure. We present a novel method for full 3D printing of crosslinked structures made from unmodified type I collagen. The methods uses only demonstrated biocompatible and most widely accepted tissue scaffold materials. Resolution of 1 ?m for both standing lines and high-aspect ratio gaps between structures is demonstrated and complex 3D structures are fabricated. High-resolution, 3D control of the fabrication of collagen scaffolds will facilitate higher fidelity recreation of the native extracellular environment for engineered tissues.

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Biological applications of silica nanosprings, a tunable 3D scaffold

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ABSTRACT

3D porous scaffolds, which are similar to nature extracellular matrices that induced synthesis of tissues and organs, are an ideal bone graft substitutes. Scaffold designs include sponges, fibers and meshes. These designs are chosen because of their biocompatibility, mechanical properties, pore size and the growth of organized cell communities. Fabrication techniques for engineering scaffolds depend almost entirely on the bulk and surface properties of the material and the proposed function of the scaffold. Most techniques involve heat, vacuum, pressure and the design of a 3D nanostructured pattern. While each material presents advantages and disadvantages, the appropriate technique must be selected to meet the requirements for the specific tissue. In some cases these materials also provide ideal characteristics for biosensor or bioreactors applications. The present work focus on a collagen-like nanomaterial that had proved to facilitate osseointegration, while being compatible with current implant technologies. Silica nanosprings are a unique nanomaterial made of pure amorphous silica with a gravimetric surface area of 400 m2/g. Figure 1 shows the macro, micro and nano morphology of this helical nanostructure which could be lithographically pattern and covalent bonded to most substrates. It will also be presented several approaches for coating substrates with silica nanosprings and surface engineer them with metal oxides, metal nanoparticles, biomolecules and combinations thereof, all with specific applications in mind. Finally, an overview of the micro-nano fabrication procedures employed in the engineering of chemical and biological sensors and reactors will be presented.

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Anodized TiO2 Nanotube Film for Controllable Drug Delivery in the Implant

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ABSTRACT

To control drug delivery is to administer the necessary amount of drug safely and effectively to specific sites in the human body and to regulate the In this study, we develop a method for controllable drug release using an innovative hybrid biodegradable polymer/TiO2 nanotube structure and drug release mechanisms are presented.

Drip Flow Photobioreactor Feasibility Test with Chlorella vulgaris

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ABSTRACT

In recent years, there has been a resurgence of concern over the harmful impacts that fossil fuels have on the Earth which has led to a renewed interest in biofuels; such as algal biofuels. In the industry, a key issue of algae growth has been low cell density which leads to high operation costs. The goal for this research project is to develop a photobioreactor that minimizes these costs, while also maximizing the algae cell density. This reactor will be developed by the students under the guidance of their faculty advisor at Miami University. The idea is that once the design and harvesting scheme have been thoroughly tested in the small scale lab, it can then be applied to real world industrial sized processes. Regardless of the success of the design, the data obtained by the research team should prove to be valuable to the field of biofuels. Since low cell density is a major problem in the industry, even a minor increase in production could lead to breakthroughs down the road. This research will help algal biofuels become a more reasonable economical option which will lead to them becoming a more reliable alternative to fossil fuels. The Chlorella vulgaris strain of algae was selected for this project for its easiness to cultivate and relatively high oil density. These goals will be achieved by developing a small scale photobioreactor as well as laboratory harvesting and testing the algae samples under different growing conditions.

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Decellularized Liver Scaffold Modeled as a Deformable Porous Material

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ABSTRACT

Tissue engineering has been applied successfully for simple structures that can be constructed using thin sheets of cells, such as bladder, skin, and arteries. Bioengineering of large solid organs, such as liver, presents greater challenges due to limited diffusion of nutrients and oxygen within the engineered tissue mass. Scaffold systems based on acellular native organs present two key advantages over synthetically manufactured scaffold materials for large solid organs: they retain the native extracellular matrix (ECM) composition and preserve the network of vascular channels. When an acellular organ scaffold is seeded with cells and the resulting bioengineered construct is developing in vitro, the cells must home to their respective niches then proliferate and fill the construct's parenchyma. It was shown in previous work that appropriate fluid mechanical stresses in the perfused scaffold are essential for cells to migrate, proliferate, and form functional tissue. However, due to the complex 3D structure of the bioengineered construct, little quantitative information is available about fluid stresses acting locally on cells seeded in perfused scaffolds, how these fluid stresses are impacted by the proliferation of cells in the scaffold over time, and how such altered fluid dynamics might impact subsequent tissue growth and function. This study reports a poroviscoelastic model to simulate the distribution of fluid stresses in developing bioengineered liver, and the correlation of model parameters to experimental measures of cell proliferation and tissue organization at different stages of in vitro tissue development.

Development and characterization of ultra dry foams for hydraulic fracturing applications

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ABSTRACT

Hydraulic fracturing is the most widely used well stimulation technique, which demands significant amount of water. Another concern is the damage that water injection might to do to producibility of some reservoirs due to clay swelling at the fracture face. Foams, dispersions of gas in liquids, are great substitutes for the contemporary fracturing fluids. They reduce water consumption, by substituting a portion of water with gas. In addition, they inherently possess relatively high viscosity, which benefits proppant transport into the fracturing zone. Further, CO2 foams reported on here are nearly incompressible and thus can deliver the designed hydraulic pressure into the fracturing zone.
In our recent work we have developed and characterized novel formulations of ultra dry foams. Using cationic and anionic mixtures (e.g. C10DMA and SLES) we tuned local curvature of the surfactants that subsequently developed worm-like micelles with enhanced stability. The foams were quite stable at high qualities within the range of 80-98%, and possessed viscosities in the range of 20-200 cP (at shear rates of 200-2000 s-1). In addition, with a different chemistry, we used EOR5 nanoparticles and LAPB surfactant mixtures to generate viscoelastic lamellae with high temporal stability and viscosities as high as 100 cP (at shear rate of 200 s-1).
Although for proppant transport high viscosity and highly stable foams are desirable, we want to make sure that upon flowback the foam does not draw the proppants back from the hydraulic fractures. To address this, we are exploring the possibility of foam destabilization by fine tuning the foam formulation. The foams produced are stable enough to carry sand proppants at high pressures, yet vulnerable to pressure reduction when they break down and leave proppants behind. For these experiments, we have collected foams in high pressure Sapphire cells and measured the settling time of proppants at different pressure, temperature, concentration, and foam qualities. In addition, we developed a multi-scale model to quantify lamella stability and strength for holding sand proppants. Lowering concentration of surfactants and increasing foam quality increased the vulnerability of the foam texture to pressure reduction and reduced the foam life-time. This susceptibility was more pronounced in the case of LAPB-EOR5 mixture compared to SLES (+C10DMA).

An Experimental Investigation of the Stability of and Oil Recovery due to Magnetic Nanoparticle-stabilized CO2 Foam in Microfluidic devices

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ABSTRACT

Magnetic nanoparticles (NPs) are used to stabilize CO2 foam for use in enhanced oil recovery (EOR) processes. Paramagnetic iron oxide NPs, with an average diameter of less than 20 nm, are coated with a silica shell, which is synthesized using FeCl2 and tetraethyl orthosilicate. The surface of silica shells is modified by using dichlorodimethyplsilane to create NPs with partial hydrophobicity. The resulting NPs are capable of being magnetized in the presence of an external magnetic field. Formability and stability of CO2 foam, stabilized with these NPs, are studied via a modified bulk foam test and experiments using microfluidic devices. Stability and formability of CO2 foam, stabilized with surface modified magnetic NPs, are quantified and compared with CO2 foam stabilized with nanoclays and silica NPs [1]. The microfluidic devices are made out of borosilicate glass and are based on a two-dimensional representation of a sandstone. The porous medium is 41mm in length and 35mm in width with 20?m deep channels. Data during microfluidic experiments is collected using an ultra-high resolution full frame image sensor paired with high-end optics, which allows the entire surface of the two-dimensional porous medium to be unobstructed for observation. Images of the entire porous medium are captured while preserving the resolution required to discern features as small as 10?m. The high-resolution images make it possible to explore foam density in the medium as a function of time, quantify foam stability and visualize multiphase flow inside the porous medium. Additionally, saturation of flowing phases and incremental oil recovery due to the use of NPs-stabilized CO2 foam are established as a function of time. NPs are recovered and recycled by applying an external magnetic field to the outflow stream. The efficacy of the recycling is quantified as a function of the strength of the magnetic field, type of oil and the porosity and permeability of the medium. Pore-scale deposition of NPs and potential permeability alteration are investigated using fluorescent dye-doped NPs.

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Visualization of Oil Displacement by Foam in Heterogeneous Porous Media

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ABSTRACT

Foams have been used in the past for vertical conformance and mobility control in gas enhanced oil recovery processes. They have the unique property to divert flow from high permeability region to low permeability region. However, this complex foam transport phenomenon is still not well understood, especially in the presence of crude oil. Understanding the different underlying mechanisms is vital to model such foam flow in heterogeneous porous media. Therefore, the goal of the present work was to gain a fundamental understanding of foam transport in such systems. An in-house, 3D sandpack holder (inner dimension: 3”x 5.5” x 1”) was designed with the front face made of a transparent acrylic sheet to visualize the oil displacement process. It was packed with two layers of silica sand — top layer with 40-70 mesh and bottom layer with 100-120 mesh, which resulted in a permeability contrast of 6:1. The system was vacuum-saturated with crude oil. Water flood with subsequent foam flood was performed using different surfactant/nanoparticles formulations. Aqueous foams were created in porous media in-situ by co-injecting the surfactant and/or nanoparticles (NP) with nitrogen gas at a fixed quality. The pressure drop across the sandpack was measured to estimate the achieved mobility reduction factor (MRF). The water flood recoveries in these cases were very low (~ 30% OOIP) due to channeling in the top high permeability region, leaving the bottom low-permeability region completely unswept. Foam flooding lead to a drastic improvement in sweep efficiency in both high and low permeability region. It resulted in an incremental oil recovery as high as 40% OOIP even under immiscible conditions. This study is first-of-its-kind to visually demonstrate the flow diversion due to foam, in the presence of crude oil, in a heterogeneous, realistic porous system. The different oil recovery mechanisms via foams were observed. Depending on the surfactant/NP type, different degree of cross-flow was observed between the two layers of sands. Such cross-flow behavior is typically not captured in the conventional foam simulators. Complementary bulk foam experiments such as Bartsch shake test, static foam tests were also performed to understand foam-oil interaction for the different formulations used. In summary, this study offers a novel systematic investigation of foam transport in heterogeneous porous media in the presence of reservoir crude oil.

Direct Visualization of Emulsions During Flow: Impact of Wall Wettability on Emulsion Stability

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ABSTRACT

Emulsion flow through restricted spaces is a fundamental process in the extraction of oil via water flooding or steam assisted methods. Moreover, reservoir wettability has a dramatic impact on the stability of emulsions as they flow through the reservoir, resulting in differences in the efficiency of the enhanced oil recovery process. In this work, both particle-stabilized and classical emulsions are directly visualized during flow using laser scanning confocal microscopy. Different wettability pores are simulated using glass capillary tubes with either a hydrophilic or lipophilic surface. Oil in water emulsions are clearly seen to exhibit stable flow through the water-wet (hydrophilic) pores, while flow instabilities are observed when using oil-wet (lipophilic) pores. Furthermore, atomic force microscope and rheological analysis provides valuable insights into the origins of these flow instabilities. These techniques indicate that the emulsion's stability during flow is dictated by the energy of adsorption between the pore-wall and emulsion stabilizer, along with the overall stability of the emulsion to sheer stress.

Modelling in-situ foam generation using a dispersed surfactant in the gas phase

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ABSTRACT

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 excellent 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 developed a mathematical model that accounts for the foamer mass transference between the gas and liquid phases in a non-equilibrium state with a particle interception model. Also, the reversible and irreversible adsorption of surfactant on the rock surface in dynamic conditions with a first order kinetic model. And, the foam generation, coalescence and transport using a population balance mechanistic model. This dispersed foam model was used in order to quantify the increase in the recovery factor and the effectiveness of a well intervention treatment with disperse foam technique.

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Two-dimensional foam flows in an analog porous medium

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ABSTRACT

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. We investigate foam flow through a two-dimensional porous medium consisting of circular obstacles positioned randomly in a horizontal transparent Hele-Shaw cell. The local foam structure is recorded in situ, which provides a measure of the spatial distribution of bubble velocities and sizes at regular time intervals. The flow exhibits a rich phenomenology including preferential flow paths and local flow intermittency/non-stationarity, despite the imposed permanent global flow rate. Moreover, the medium selects the bubble size distribution through lamella division-triggered bubble fragmentation. Varying the mean bubble size of the injected foam, its water content, and mean velocity, we characterize those processes systematically. In particular we measure the evolution, along the flow direction, of the distribution of bubble sizes, and analyze the efficiency of bubble fragmentation as a function of the control parameters. The bubble fragmentation can be modeled numerically and to some extent analytically, based on statistical measures inferred from the experimental data. The resulting direct model is compared to the data with an excellent agreement. We also show that the distributions of bubble sizes and velocities are correlated, and discuss the implications in terms of foam rheology.

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Transport behavior of a nanoparticle-stabilized foam

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ABSTRACT

Foam injection into the subsurface is performed to improve gas control mobility for residual oil extraction in, e.g., enhanced oil recovery and contaminated site remediation. Foam improves the gas mobility control as the gas viscosity is increased through its dispersion into a liquid phase. Finer the bubbles the lower the gas apparent viscosity (or foam viscosity) and the better is the sweep efficiency of the residual oil. A chemical surfactant adsorbed at the gas-liquid interface is generally used to maintain an optimal foam texture (number of bubbles for unit volume) however it can be desorbed making the foam coarser.
Here, we present an experimental and modeling study on the effect of nanoparticles on foam stability. Nanoparticles are adsorbed onto the bubble interface irreversibly and therefore they are expected to keep the desired texture of the foam for the entire time of its application. In this study, we use silica nanoparticles in conjunction with a surfactant to study the transport behavior of a CO2 foam in a porous medium. Experiments were performed using a glass-bead pack and Boise sandstone with foam quality (fg) 0.1-0.9 until steady-state. Foam flow was described by a mechanistic population balance model coupled with the fractional flow equation and constitutive equations for foam generation and destruction based on lamella division and bubble coalescence mechanisms, respectively. In order to minimize the uncertainty, model parameters were estimated by combining experimental data of pressure gradient during steady-state and transient.
Experiments and theory agree very well and the overall results show a significant increase in foam texture and stability when nanoparticles and surfactant are added to a foam flow in a low permeability porous medium. Data from tests with various nanoparticle concentrations (cn) show that gas apparent viscosity changes with fg and cn. But its optimal value does not vary with cn and it is already attained at fg equal to 0.8 when 0.01 wt.% of nanoparticles are added together with 0.04 wt.% of surfactant. Employing 0.04 wt.% of surfactant under conditions of temperature, salinity, and permeability comparable to a deep formation, foam viscosity is approximately 4·10-2 Pa·s, and increases of one order of magnitude when only 0.1 wt.% of nanoparticle is also added.

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Parametric study of a model to describe foam displacement for isotropic and anisotropic heterogeneous systems

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ABSTRACT

Foams are among the displacing fluids used to improve percentage of production during oil extraction processes in tertiary recovery techniques. Oil reservoirs are porous rock formations where surfactant and gas are injected to form foam and help to displace oil. Therefore, it is important to investigate how foam flows inside oil reservoirs, taking into account the characteristics of the porous medium. Many studies of foam motion assume that the reservoir is homogeneous. However, in real fields, heterogeneous conditions are found, and these are the systems of interest in this study.
We use a model for foam rheology known as pressure-driven growth [1, 2]. Assumptions of this model are that the foam motion is driven by a pressure difference between the hydrostatic pressure inside the reservoir and the injection pressure, which focuses on a wet foam region between the aqueous and gas phases. This zone, the foam front, can be represented by a one-dimensional line in a two-dimensional system.
The mathematical representation of the model is simple but the numerical solution of the system presents some challenges. One of the issues is that spurious results are obtained when the foam presents concavities. In the heterogeneous case, concavities are expected to develop.
It has been shown [2] that concave regions can be propagated with similar equations for pressure-driven growth, but applying a correction factor for their velocities. This factor depends on whether the system is isotropic or anisotropic. Once the problem with the propagation of concavities is handled we are now interested on how the parameters that influence the level of heterogeneity affect the system and influence the foam motion.

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New insights on foam rheology in porous media

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ABSTRACT

Due to their large potential in boosting EOR gas flooding, foams are currently a matter of active work at both laboratory and pilot scale[1-5]. Nevertheless, major uncertainties remain regarding the actual physics underlying the rheological behavior and transport of foam in porous media. Foams may exist in two distinct states in porous media: weak and strong. Strong foams presents two flow regimes (low and high quality) depending on the foam quality (volumetric gas fraction fg). The transition occurs at a given fg (fg*), where maximum pressure drop is achieved. It is widely accepted that strong foam low quality regime exhibits shear thinning behavior. Conversely, no consensus has been achieved for the high quality regime, as diverse behaviors have been reported in the literature, most probably due to the instability of foam in this regime[2,3].

The present work aims to advance the understanding of the physics underlying the rheological behavior of foams in porous media and to question the aforementioned admitted properties. To this end, we performed a systematic experimental study of the impact on foam apparent viscosity (μfapp) of the following main parameters: foam quality, interstitial velocity, initial permeability, and pore pressure. The experiments were done in sandstone cores at 60°C, using synthetic desulfated seawater (DSW) as injection brine and a proprietary surfactant formulation. The gas used was a mixture 4:1 of CO2/CH4. Foams were generated in-situ by co-injection of gas and surfactant solution.

Our results showed that fg* was almost independent of interstitial velocity and varied linearly with the reciprocal square root of the permeability. The impact of pressure was evaluated for multiple fg's at a single interstitial velocity in one core. The relative permeability of gas in presence of foam increased almost linearly with pressure. All data fitted a single curve regardless the fg.

An in-depth investigation of the rheological behavior of foam in both flow regimes and under a range of permeability and foam quality was performed at constant pore pressure. Interestingly, the shear thinning behavior of foam (independently of fg, of permeability and flow regime) could be described by a master curve of μfapp as a function of shear rate that obeys a power law with a universal exponent of -2/3. If only the shear thinning data in the low quality regime was considered, the same power law dependence was observed, but with an exponent of -3/4.

Such correlations hold great potential to advance the physical modeling of foam flow in porous media and to improve the Foam-EOR process modeling in the reservoir simulators, which are mostly based on the "steady state" phenomenological model, with limited predictive abilities.

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Effects of pore connectivity on foam flow in porous media

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ABSTRACT

Understanding of foam flow in porous media is of great importance to various real-world applications such as soil remediation and enhanced oil recovery. Foam injection in porous media proved to be a promising approach to address the problems of viscous instability and gravity override during oil displacement in porous media. Foam is relatively immobile in porous media due to the forces that are required to drive foam films through the channels in a porous medium. This relative immobility of foam helps to suppress the fingering phenomena that would otherwise occur, leading to a more uniform displacement of oil from the reservoir (Grassia et al., 2014). Despite many advances in understanding of foam flow in porous media, fundamental understanding of the parameters influencing foam dynamics in porous media is still missing due to the complexity of the problem at various length scales. Many factors influence foam flow and its sweep efficiency in porous media including the type of surfactant used to make foam, surfactant concentration, foam texture, quality and stability, pore size distribution and heterogeneity of porous media together with the properties of the displaced fluid residing in the porous medium (Kovscek and Radke, 1993; Mas-Hernandez et al., 2015; Osei-Bonsu et al., 2016).
There are many open questions required to be answered for an accurate prediction of foam flow and its sweep efficiency in porous media. For instance, any porous medium, no matter how homogeneous, still contains a degree of heterogeneity and how these heterogeneities influence foam performance is not well-understood. On top of that, foam behaves differently in the presence of different fluids. For example foam stability is altered depending on oil properties residing in porous media (Osei-Bonsu et al., 2015) influencing its mobility. This adds to the complexity of the problem at pore and macro-scale. Motivated by the importance of foam flow in porous media, the specific objective of this work was to delineate the effect of pore connectivity on the dynamics of foam flow in porous media. To accurately control pore connectivity, we have designed various porous media with well-defined pore connectivity and aspect ratios which were used to manufacture the porous medium using state-of-the-art 3D printing technique. Using time-lapse imaging, we have conducted a comprehensive series of experiments using 2D polymeric printed porous media with the coordination umber of 3, 4 and 6. The foam flow with well-controlled properties and injection rates in porous media was recorded with a high resolution CCD camera. The obtained images were analysed to delineate the dynamics of foam flow in porous media. The results enabled us to determine how the coordination number influences the morphology, patterns and sweep efficiency of foam flow in porous media at both bubble-scale and macro-scale. Using printed porous media with well-controlled pore geometry and coordination number in our experiments extended our fundamental understanding of foam flow in porous media.

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Stability of foam during oil displacement in porous media

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ABSTRACT

The relative immobility of foam in porous media suppresses the formation of fingers during oil displacement leading to a more stable displacement which is desired in various processes such as Enhanced Oil Recovery (EOR) or soil remediation practices (Khatib, 1988; Grassia et al., 2014; Osei-Bonsu et al 2015). However, the success of foam application is hampered by the low stability of foam in the presence of oil. Many experimental studies have reported the detrimental effects of oil on stability of bulk foam (e.g. Osei-Bonsu et al 2015). The destabilizing effect intensifies as the hydrocarbon chain length, viscosity and density of the oil decreases. Although such effects were studied and observed in bulk foams, there is much less information about how foam behaves in porous media in the presence of oil. Motivated by the importance of foam stability in various applications including oil recovery and soil remediation, the specific objective of the present work was to delineate the relative importance of the foam characteristics, the type of oil and pore size of porous media on the stability of foam during oil displacement. We conducted a systematic series of experiments using Hele-Shaw cell and sand-packs to investigate the effect of two foam qualities, three oils and two porous media with well-defined particle size distribution on the stability of flowing foams. The Hele-Shaw cell and sand-packs were initially filled with oil and then foam was injected through the cell in order to displace the oil. An automated camera was used to capture the evolution of the displacement process at defined time intervals. Images from the camera were analysed using Image J software to determine the effects of the above parameters on the breakthrough time, front propagation velocity and bubble size distribution in the vicinity of the oil. Our results extend our understanding of the effects of different parameters on the stability of foam while flowing in porous media in the presence of oil.

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Numerical solution of plate poroelasticity problems

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ABSTRACT

We consider the numerical solution of boundary value problems for poroelastic plates. The basic system of equations consists of the biharmonic equation for vertical displacement and nonstationary equation for pressure in the porous medium [1, 2].
The computational algorithm is based on the finite element approximation in longitudinal coordinates [3] and the finite difference approximation in time [4]. We formulate standard stability conditions for two-level schemes with weights. The computational implementation of such schemes is based on solving a system of coupled equations: fourth-order elliptic equation for displacement and second-order elliptic equation for pressure.
We construct unconditionally stable splitting schemes with respect to physical processes, when the transition to a new time level is associated with solving separate problems for the desired displacement and pressure. The stability of the scheme is achieved by passing to three-level difference scheme and by choosing a weight used as a regularization parameter [5, 6]. We present stability estimates of the schemes and provide numerical experiments supporting the derived estimates.

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Measuring relative in-plane diffusivity of thin and partially saturated porous media

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ABSTRACT

A new experimental technique, extended from similar work on dry materials, is presented for measuring the relative in-plane di?usivity tensor components for partially saturated porous media. The method uses the transient response to a change in oxygen concentration at the boundaries of a thin porous sample held between two ?at plates. The custom-built holder is kept close to the freezing temperature of water to ensure constant saturation throughout the experiment. Fick's second law is used to ?t the transient change in concentration to an analytical solution in order to obtain the di?usion co-e?cient for samples of di?ering saturation. As expected the e?ective diffusivity was found to decrease with increasing saturation of the media as the porosity of the media is reduced and the tortuosity of the diffsion pathways increase. The relative in-plane diffusivity of some common fuel cell gas di?usion layer materials are found to follow a power-law function dependent on the saturation consistent with previous modelling work. The advantage of the proposed method is the direct measurement and relatively simple and inexpensive experimental set-up.

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Validation of Two-Phase Flow in a Pore Network Model Simulation using a Scaling for Percolation in Thin Porous Materials

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ABSTRACT

Validation of numerical simulations of percolation in thin porous materials is challenging due to the scholastic nature of the material and flow as well as the absence of a representative volume in the through plane direction. In this work a characterization experiment, a numerical model, and a scaling of percolation is described that enables validation of the numerical model for thin porous materials. A Hele-Shaw experimental setup is used to measure the pressure required to inject water in a thin porous material. Simultaneously to the pressure measurement, the water distribution is recorded using video imaging. The new scaling is defined by combining both, the pressure and the water distribution occurring during the percolation. Parallel to the experimental effort, a numerical pore network model has been developed to simulate the drainage percolation observed in the Hele-Shaw experiments. The scaling of the flow is applied to the results of the numerical simulations following the same procedure used with the experimental data. The numerical and experimental data are quantitatively correlated for percolation occurring in multiple, distinct thin porous materials.

Numerical Modeling of Flow in Highly Porous Thin Fibrous Materials using Pore Topology Method

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ABSTRACT

Thin, highly porous materials are ubiquitous in nature and widely employed in many products and devices. Examples range from living tissues, filters, membranes and absorbent materials to fuel cells and microfluidic devices, driving the need to better understand the structure and processes in these materials. Their distinct properties, however, present new challenges in experimental and numerical characterization. Thin, highly porous materials are characterized by thickness on the order of pore dimension, and by porosity of larger than 60%. Furthermore, large, irregular pore spaces preclude easy characterization of the pore space geometry.

Pore Topology Method (PTM) is a recently developed micro-scale modeling technique to simulate flow in porous media. The core concept of PTM is to reduce the complexity of the 3-D void space geometry by employing its medial surface as the solution domain; hence, PTM provides a simple, topologically consistent and fast methodology to simulate flow in porous materials.

In this talk, we present our results for quasi-static single phase and two-phase flow in a series of real and virtual thin fibrous materials with a wide range of porosities. Despite simplicity and low computational cost, PTM results are in excellent agreement with currently available analytical and numerical approaches, as well as experimental data. We further report our progress on incorporation of solid matrix swelling in PTM simulations.

Drying salt solutions in capillary porous media: a discrete modeling approach

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ABSTRACT

Salt crystallization in porous media during drying is a common phenomenon in conjunction with several natural and industrial applications, such as soil physics, protection of cultural heritage, underground sequestration of CO2, etc. In this work, a three-dimensional pore network model (PNM) has been developed to simulate the dynamics of salt transport and crystallization in capillary porous media during the drying process. In order to represent the porosity of porous materials accurately, the void space has been modeled by bundles of uniform capillaries (instead of single throats in our previous crystallization PNM). The radius of these capillaries varies between each bundle; it can be generated by sampling from a pore size distribution which is either given analytically or determined by experiments. Simulations are run for various pore size distributions as well as various process conditions (such as drying rate and the initial concentration of salt). In this study, we also aim to investigate one of the main issues observed in simulations with two-dimensional pore networks, namely the reproducibility of the results. This issue is a result of the randomness of the pore sizes between different simulations, and it brings up the following question: which network size can be considered as representative to minimize the variance of the results? In order to properly answer this question, a series of Monte-Carlo simulations have been conducted where the size of the network was varied to obtain the representative size of pore networks for mono-modal and bimodal pore size distributions.

Darcy’s law for flow in a periodic thin porous medium confined between two parallel plates

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ABSTRACT

There exist several mathematical approaches, collectively referred to as homogenization theory, for deriving Darcy's law for an incompressible viscous fluid flowing in a porous medium. The present work is devoted to the multiscale expansion method which is a formal but powerful tool to analyze homogenization problems.

Constructing asymptotic expansions for velocity field and pressure in the incompressbile Navier-Stokes system, we derive Darcy's law for a thin porous medium (TPM) which can be described in terms of two small parameters: the interspatial distance between obstacles ε and the thickness of the domain μ. More precisely, we consider pressure driven flow through a periodic array of vertical cylinders confined between two parallel plates. A representative elementary volume for such TPM is a cube of lateral length ε and vertical length $\mu.$ The cube is repeated periodically in the space between the plates. Each cube can be divided into a fluid part and a solid part, where the solid part has the shape of a vertical cylinder (of length μ). Pressure driven flow within the plane of a confined thin porous medium takes place in a number of natural and industrial processes. This includes flow during manufacturing of fibre reinforced polymer composites with liquid moulding processes and passive mixing in microfluidic systems.

Boundary value problems involving several small parameters are delicate to analyze as letting the parameters tend to zero at different rates may cause different asymptotic behavior of the solutions. Therefore one must distinguish three kinds of TPM whether ε tends to zero slower, faster or at the same rate as μ:
\begin{description}
\item[VTPM] Very Thin Porous Medium is characterized by $\mu \ll \varepsilon.$ The cylinder height is much smaller than the interspatial distance.
\item[PTPM] Proportionally Thin Porous Medium is characterized by $\mu\sim\varepsilon.$ The cylinder height is proportional to the interspatial distance with $0<\lambda<\infty$ denoting the proportionality constant, i.e. $\mu=\lambda\varepsilon.$
\item[HTPM] Homogeneously Thin Porous Medium is characterized by $\mu \gg \varepsilon.$ The cylinder height is much larger than interspatial distance.
\end{description}

In all three cases the asymptotic behavior is governed by a two-dimensional Darcy law, where the permeability is found by solving local boundary value problems, so called cell problems, that do not involve ε nor $\mu.$ However, the local problems are different in each case. In the intermediate case (PTPM) the cell problems are three-dimensional and the coefficient of proportionality λ appears as a parameter in the equations. In the extreme cases (VTPM and

HTPM) the cell problems are two-dimensional, which is a considerable simplification compared to the intermediate case. VTPM and HTPM can also be considered as limiting cases of the intermediate case. Indeed, if permeability $K^\\lambda$ is regarded as a function of $\\lambda$ and
\begin{equation*}
K^0=\lim_{\\lambda\to 0} K^\\lambda,\quad K^\\infty=\lim_{\\lambda\to \\infty} \\lambda^{2}K^\\lambda
\end{equation*}
then K^0 and $K^\\infty$ are the permeabilities corresponding to VTPM and HTPM respectively. This relation is confirmed both theoretically, by constructing asymptotic expansions in $\\lambda,$ and by solving the cell problems numerically.

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A review of Two-Phase Flow Models for Thin, Swelling Porous Media

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ABSTRACT

Understanding fluid flow and deformation processes in thin swelling porous media is critical for developing superior consumer absorbent hygiene products such as wipes, paper towels, feminine pads and diapers. Fluid-flow models have proven very valuable for the development of these products and have led to the development of fundamental understandings in transport mechanisms, numerical simulation tools, computation infrastructure and lab methods for both characterizing absorbent materials as well as validation of flow and deformation models.

In this talk, we will present the fundamental equations governing liquid absorption and solid deformation during the unsaturated two-phase flow of liquids in thin, swelling porous media under isothermal conditions. The resulting model equations will consist of balance equations combined with a series of constitutive relationships. The need for advanced and efficient numerical methods to solve the flow, absorption and deformation processes in these thin porous media will be discussed. We will present some methods to convert the full 3-D flow and deformation model into the equivalent 2-D ones in order to improve the computational speeds.

Pore-scale imaging and modeling of water-based ink setting and drying process on coated paper

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ABSTRACT

A high quality print using the inkjet technology of printing is designed by considering both the ink properties and the paper characteristics. The paper porosity, permeability, thickness/bulk, sizing and capillary structure are the most important control parameters in designing inkjet print surfaces, from the point of view of ink spreading and penetration. Inkjet coatings (with a thickness around 10 μm) traditionally have used silica pigments with their combination of high porosity micropores and high surface area, providing rapid ink drying. In this work, we investigate the effect of porous structure of the coating layer on penetration and spreading of ink during inkjet printing process. We adopted a nano-tomography and pore-network ?ow modelling approach. The pore structure of the coat layer of a glossy paper sample was extracted using Focused Ion Beam milling and Scanning Electron Microscope (FIB/SEM) imaging, with a resolution of 6.25 nm. The resulting image was used to construct a realistic pore network, which is then used in a dynamic pore-network model for two-phase flow. We determined the pore size distribution, porosity, capillary pressure-saturation curves, and relative permeability for the coat layer. Dynamic imbibition simulation were performed to find out more about the imbibition process, vertical and horizontal penetration of ink during printing.

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When ink meets porous paper: briefing on the involved physical processes

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ABSTRACT

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 department 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 printing with aqueous ink with polymeric particles. Understanding 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 presented; the main focusing will be on: a) water evaporation from inks as thin films and droplets, b) absorption of the liquid by porous paper, c) drying of the printed ink. The influence of both the liquid physical properties and the paper characteristics will be considered.
Methods of investigation will be briefly presented, including their strengths and limitations.

Stochastic Fiber Network Models for Paper: Generation, Deformation, Deformation Dependent Permeability

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ABSTRACT

The liquid transport in porous fibrous materials, like paper, paperboard and membranes, is influenced by (a) the microstructural properties of the base material, (b) the reshaping during the manufacturing process, and (c) the deformation due to storage and conditions of use. As typical application one can have in mind the life cycle of a coffee filter paper.
We present a microstructure simulation method for the prediction and optimization of functional properties, e.g. permeability, where large local deformations of realistic 3D fiber networks are captured in contrast to similar approaches. These local deformations lead to significant changes of the pore space, and therefore the fluid flow through the pores is changing strongly.
The generation of virtual microstructures, sometimes called fiber networks, and their discretization on regular meshes is explained. Then an efficient numerical solution method for the nonlinear elasticity problems in fiber networks is presented. Numerical tests show the dependence of resulting macroscopic properties from the magnitude of mechanical deformation.

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POC Blood Coagulation Diagnostics Using Paper-Based Lateral Flow Device

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ABSTRACT

Cardiovascular disease is a leading cause of death world-wide [1]. Physiologically, blood coagulation rapidly limits blood loss from a damaged vessel, which is critical for healthy individuals [2]. For many patients, however, inhibition of blood coagulation using blood-thinning medication (anti-coagulants), such as heparin or warfarin, is required to reduce the risk for stroke, pulmonary embolism, heart attack and other life-threatening cardiovascular diseases. Regular lab monitoring during anticoagulation therapy is required and usually performed by trained specialists in clinical settings. The goal of our research is to develop a paper-based point-of-care (POC) lateral flow assay (LFA) device that can be used by patients in home setting to monitor their blood coagulation ability.

We utilize LFA structure for the device – sample pad, nitrocellulose membrane and wicking pad are supported by plastic backing and placed in cassettes, as shown in Figure (a). Unlike traditional LFA assays, our LFA device does not involve any chemicals but solely rely on the filtration and porosity properties of different strip components.

Various blood coagulation abilities are achieved by adding Ca2+ ions to stored rabbit blood in which normally present Ca2+ ions are immobilized by citrate in order to prevent coagulation. By externally adding Ca2+ ions back we reactivate the blood coagulation cascade. In simple terms, the more ions are added the stronger the blood coagulation ability becomes, which means “thicker” blood. The travel distance of red blood cells (RBCs) in the nitrocellulose membrane is used as a natural indicator of coagulation ability – shorter distance indicates thicker blood and vice versa. As shown in Figure (b), our LFA device is able to detect various coagulation ability achieved by different calcium concentration in citrated rabbit blood.

The distance of the RBC front is found to decrease linearly with increasing Ca2+ concentration, with a travel rate decreasing from 3.25 mm min?1 for no added Ca2+ to 2.2 mm min?1 for 500 mM solution. Compared to conventional plasma clotting analyzers, our LFA device is much simpler and it provides a significantly larger linear range of measurement. Using the red colour of RBCs as a visible marker, this approach can be utilized to produce a simple and clear indicator of whether the blood condition is within the appropriate range for the patient's condition [3].

Clinical trials on patients during warfarin anti-coagulation therapy were also performed and the results

are shown in Figure (c). Clinically, the international normalized ratio (INR) is used to measure patients' blood coagulation ability. Higher INR number indicates blood is thinner, and vice versa. An increase in RBC travel distance with increasing INR was observed among patients with a normal haematocrit concentration of 40%.

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Self Powered Electrochemical Urine Sensor on Paper Substrate

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ABSTRACT

In this work, we report on the operation of an electrochemical (EC) cell fabricated completely on paper substrate and powered by urine. Paper-based microfluidics provides a novel system for fluid handling and quantitative analysis for a diverse range of potential applications [1]. It is ubiquitous, low cost, easy to use portable platform, available in different pore size, textures, providing options for easy implementation in versatile applications [2]. The progressive increase in the use of paper as a prime component in immunoassays, lab-on-chip devices are the result of its excellent fluid handling capability and natural microfluidic flow within the polymer matrix without external stimulus[3].
Urine is a treasure trove of information about the human biological system. Its analysis provides very useful information about the health status of the individual. Urine-based EC cell can also be built into diapers where it can function as power indicators that provide an alert to the volume and properties of the urine produced. The electrochemical approach converts chemical potential energy of a metal into electrical energy, through oxidation-reduction (REDOX) reaction generates output potential, and catalyzes movement of electrons from one element to another thus resulting in output current. The primary operational components chosen for this device, namely electrodes, electrolytes and salt bridge are Al|NaOH|NaCl|CuSO4|Cu. Aluminum, along with being an efficient anode material with lower atomic weight (26.98), high theoretical energy density (8.1 W•h/g), high negative standard potential (-1.676V, SHE, 25°C), is quite abundant and relatively inexpensive. Its electrochemical dissolution, in addition to generating high oxidation potential, transmits three electrons per cell thus delivering reasonable high current to the load.
In this work, a multi-layer sandwich design has been utilized, with separate fabrication step for each layer: base layer (NaOH), hydrophobic layers, hydrophilic paper layer, CuSO4 strip, NaCl strip, Cu and Al electrodes. Immobilization of recognition species effectively could be achieved by physically entrapping the target material within the polymer matrix. The final cell is subsequently assembled and laminated, as shown in Fig. (a). Among primary ionic species present in urine, concentration of Na+ and uric acid (C5H4N4O3-) specifically contributes to its electrical property [4]. A single cell device (40 mm ? 30 mm), upon exposure to artificial urine volume of ~ 0.25 mL, generates open circuit voltage > 1V and short circuit current of 1 – 1.65 mA for ~ 1 hr. Figs. (b) and (c) show discharge characteristics. A twin cell device operated in series generates power to operate an LED for ~ 40 min, which can serve as the indicator of the presence of urine. The sensor selectively responds to K+ ion discharged within physiological range (25 -125 mEq/L). Single cell device generates short circuit current in range: 2.4 mA – 3.3 mA for multiple concentration ranges of K+ ions (50, 125, 130 mEq/L) in urine.

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Absorption of picoliter droplets by thin porous substrates

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ABSTRACT

Absorption of 10-50 picoliter (pL) droplets into porous substrates is studied experimentally and numerically. Behavior of droplets landing on a substrate is driven by spreading, wetting, absorption, wicking, and evaporation. In the case of pL droplets, these physical phenomena develop at different time scales: spreading and wetting at microseconds, absorption and wicking at milliseconds, and evaporation at seconds. Therefore, one can decouple these processes to minimize the complexity of the study while still capturing the relevant physics. Our study has shown that absorption of droplets by paper-like substrates can be divided into two stages. During the first stage - the liquid is absorbed by the capillary forces and the droplets disappear from the substrate surface. This is a typical spontaneous imbibition of wetting liquids into porous media. During the second stage – continuous diffusion (wicking) – the liquid continues to spread inside the medium until an equilibrium state is reached. The second stage is much slower than the first one. A high-speed imaging system is capable of visualizing individual droplets impacting, spreading, and absorbing (disappearing) on substrates at rates up to 1 million frames per second. To simulate droplet dynamics, Navier-Stokes equations coupled with Darcy's equation are solved using the commercial code FLOW3D. The time-dependent droplet shape extracted from numerical simulation is in good agreement with that captured by the high-speed imaging system. The effect of drop impact velocity and fluid properties on final dot shape in the porous substrates is investigated through a series of parametric computational fluid dynamics simulations.

An optical method for measuring strain induced by swelling in hydrogels

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ABSTRACT

An optical method for measuring strain induced by swelling in hydrogels
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Hydrogels have been the subject of extensive theoretical and experimental studies for the last fifty years. The excellent water uptake of hydrogels has been the driving factor for this attention. This characteristic has made hydrogels interesting for a wide range of applications in biomedical and pharmaceutical industries [1]. The relation between swelling and mechanical properties of hydrogels is of vital importance for most of these applications. In this work we studied the relation between swelling and the mechanical characteristics of hydrogel. We have used, for the first time, three dimensional micro-particles tracking velocimetry (3D-µPTV) to measure the strain of a swelling gel [2]. The result obtained using this method could be used to validate theoretical models developed to predicts strain of swelling hydrogels [3].

Figure 1: (Left) a picture of a gel particle doped with fluorescent micro-beads. (Right) a picture of a sample cell with the gel particle inside it.

For measuring strain, gel particles (size between 200 µm to 800 µm) were doped with 2 µm-diameter fluorescent beads as shown in Figure 1 (left). The doped particle is placed inside a flow cell. Figure 1 (right) shows a picture of the flow cell and the gel particle inside it. When water is let inside the flow cell the gel starts to swell. The 3D-µPTV setup is used to trace the positions of the fluorescent beads as the gel is swelling. The positions of the fluorescent beads as a function of time is used to determine the strain inside the gel.

Figure 2 (a) shows a top and a cross-sectional view of fluorescent particles tracks inside the gel bead, respectively. Each color represents a track of an individual bead. The track contains information about the particles positions as a function of time. The result shown in Figure 2 was measured after 50 s of the start of the swelling and measurement duration lasted for 210 s. The evolution of the positions of particles inside the gel as a function of time will be used to determine the local finite strain in the gel in 3D.

(a) (b)
Figure 2: Top (a) and cross-sectional (b) views of tracks of individual particle inside a gel particle.

In this study we have developed a method to quantitatively describe swelling of hydrogels in 3D. The

measurement result will be used to determine the mechanical strain induced by gel swelling.

Acknowledgment

This work is support by the Dutch Technology Foundation STW, the technological branch of the Netherlands Organization of Scientific Research NWO and the Ministry of Economic Affairs under contract 12538 Interfacial effects in ionized media.

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Transport of complex mixtures in porous materials, an experimental study using NMR imaging

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ABSTRACT

On the recent United Nations conference on climate change in December 2015, the participating nations came to an agreement to keep the worldwide rise in temperature below 2 °C. This obviously impacts the use of fossil fuels and countries will aim for carbon neutrality by the second half of this century. However, this will also impact the use of materials, processes and solutions, and finding 'greener' replacements is an ongoing challenge. This also applies to our daily activities such as printing, for example, a PhD thesis, an article to read or a conference program. In the printing industry, the search to reduce the volatile components in ink has led to the development of water-based inks, which is a complex mixture containing among others water, a co-solvent such as glycerol and particles. We aim to better understand the imbibition of these complex mixtures in paper and understand how far each component penetrates in order to improve the water-based inks today and in the future.

In this research we investigate the behavior of water-based mixtures that penetrate in a porous material by using NMR (Nuclear Magnetic Resonance) measurements complemented with Rheology and DVS (Dynamic Vapor Sorption) measurements. In first approximation we use Al2O3 samples as a well-defined model for paper to quantify the penetration of each component. We investigated the dependence of glycerol and particle concentration in water on the penetration speed, and quantify to what extend the mixture separates in the porous material. We visualize the water, glycerol and particle profiles as a function of time and take advantage of the differences in T2 relaxation times to distinguish each component. Furthermore we link the behavior of our complex mixture to the rheological properties. Finally we investigated the effect of pore size on the imbibition behavior.

We found that water-glycerol mixtures penetrate into the porous material as a single liquid without splitting of the front in 200 nm, 1.1 ?m and 16 ?m porous Al2O3. Furthermore we found that the imbibition process can be governed by a modified version of Washburn's equation and that the behavior can be scaled with liquid and media parameters to result in one generic curve. To move to inkjet inks we have extended the study with Fe2O3 particles that are roughly the same size as inkjet pigment and studied their progress in the Al2O3 samples. We found that the particles can influence the liquid uptake behavior depending on the particle concentration and the interaction with the porous material.

Scanning Electron Microscopy and Spectroellipsometry to investigate paper porosity

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ABSTRACT

The penetration of liquid in porous materials has been the subject of many publications in the last decades, both theoretical understanding and sustainable industrial applications being the driving forces for these studies. Nowadays, the inkjet is one of the main printing technologies, offering the flexibility of digital printing at a breakthrough cost price, while delivering good print quality.

The quality and the robustness of a print are determined by the ink and media properties. The interactions between the ink components and the porous paper are also important. Processes as water evaporation and ink penetration into the media are vital when printing with water based inks. Concerning the liquid penetration into porous paper, it is known that both the surface and internal structure of paper have a tremendous influence. Therefore, information concerning the porosity, as well as, the pores‘ dimensions and shapes is needed for a better understanding of the processes involved.

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 mercury intrusion. The limits of the SE method are also discussed.
The method of scanning electron microscopy (SEM) is used in our study to qualitatively analyze the paper porosity at the surface and in the transversal cross-section obtained by ion polishing. Different types of plain and coated paper are investigated by the SEM method. Moreover, the SEM method is used to study the effect of the liquid penetration into paper. Changes in fibers’ dimensions as well as in pores’ shapes are revealed by comparing the SEM images of the paper before and after the liquid penetration.

Qualitative blood coagulation indicator using Radial flow assay device

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ABSTRACT

Paper-based microfluidic systems as low-cost, portable, and easy to use analytical platforms for assays, represents a rising technology, particularly relevant to improving the healthcare and disease screening especially for those areas with no- or low-infrastructure and limited trained medical and health professionals [1]. In terms of this application, paper-based microfluidic devices can be categorized into two groups, first on-demand devices, depending on the samples to be tested, the detection reagents apply in to device prior or after the test. Second is ready-to-use devices, based on particular detection these devices are designed for, by incorporating indication reagents into detection zones of the devices [2]. Conventional paper-based assay devices utilize unidirectional lateral flow (LFA) in narrow rectangular cellulose membranes. Radial flow assay (RFA) use circular membrane geometry wherein the fluid flow direction is radial. Blood samples are dispensed into the device that is laminated with self-adhesive plastic lamination sheets. Sealing the membrane minimizes fluid loss from evaporation, while placing vent openings to prevent pressure build-up, optimizes the blood-membrane interaction by controlling the transport rate. Citrated rabbit blood is used for experiments. Ca+2 as a coagulant factor is added to the citrated blood in the form of CaCl2 solutions at different concentration to mimic coagulant abilities in vitro [3]. Autonomous plasma separation occurs due to the porous nature of the cellulose membrane. The red blood cells (RBCs) travel distance decreases linearly with increasing CaCl2 concentration due to changes in blood viscosity during coagulation. RFA devices display several advantages over their LFA counterparts: shorter test time with faster flow rate, a simpler structure to fabricate, and optimization of the flow profile by eliminating the edge effect sometimes present in lateral flow geometry. From the photograph in Fig. 1 it can be clearly observed that by increasing the amount of CaCl2 concentration the RBCs travel distance (over a fixed time) decreased. This behavior shows the effect of Ca+2 ions from the added CaCl2 solution on blood coagulation process in RFA devices and the overall process shows the potential of the device for blood coagulation screening.
RBC travel distance decreases linearly with increasing CaCl2 concentration with change of blood viscosity during coagulation, as shown in Figs. 2 and 3.
Figure 4(a), shows the distance relationship between blood samples by adding CaCl2 with various concentrations. Unlike what is observed from RBC, plasma flow rate doesn't decrease significantly with more Ca+2 ions are added. The linear relationship of (travel distance)2 vs time for both blood components, shows they follow the Washburn equation[4].

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OLED as Integrated Light Source for Quantum Dot Fluorescent Lateral Flow Immunoassay

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ABSTRACT

In this project, the focus is on research to create a sensitive, quantitative, cheap & disposable lab on chip (LoC) system. Such a system has been realized by integrating organic optoelectronics and RF power sources with paper-based microfluidic systems. Paper-based microfluidic systems by themselves have several desirable characteristics, such as an integrated capillary pump, natural filtration, at the same time being cost effective and disposable1. Lateral flow immunoassays (LFIAs) are widely applied paper microfluidic systems and hence chosen as the research vehicle for this work2. Organic light emitting diodes and photo-diodes (OLEDs & OPDs) have been integrated as optical components in LoC systems by several research groups and hence its integration with LFIAs will create a device for point of care applications3.
Green phosphorescent OLEDs emitting at 520 nm were fabricated on plastic substrates. The OLED with structure, ITO/NPB/CBP:Ir/BCP/AlQ3/LiF/Al, was integrated on-chip to excite the test line of LFIA devices as depicted in Fig (a).
Antibodies conjugated with CdSe/ZnS QDs emitting at 655nm were used for the fluorescent LFIA with a simple antibody-antibody based immunoreaction scheme. For comparison of sensitivity, conventional Au nanoparticle (Au-NP) based LFIA with same immunoreaction principle was used. Integration of the OLED and color filters with the analytical membrane was achieved using simple adhesive techniques facilitated by planar nature of the layers, which suggests possible large scale manufacturing using roll-to-roll processing. The integrated device utilizes a backing membrane as the support on which various layers are placed sequentially. The concentrations of the conjugates was varied from 1nM to 100nM.
Comparisons between the emissive QD-OLED and reflective Au-NP LFIA at several conjugate concentrations are shown in Fig (b). Using grey scale contrast plots, the S/N ratio is calculated and plotted for various concentrations and the concentration at S/N of 3 was chosen from LoD values. As seen in Fig (c), the QD-based LFA had a ~7x lower LoD value than the Au-NP LFIA4

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Experimental and Numerical Studies of Pore-Scale Multi-Phase Flow

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ABSTRACT

Micro-fluidic experiments and pore-scale simulations have become important tools in studying multiphase flow in porous media. At the same time, many pore-scale numerical models lack rigorous validation and verification, and micro-fluidic experiments are hard to reproduce due to physical instabilities and challenges in precisely controlling the experiments.
We performed a set of microcell experiments and determined conditions necessary to obtain reproducible pore-scale evolution of the fluid-fluid interfaces during both infiltration and drainage phases.
Next, we modeled the experiments using Finite Volume and Smoothed Particle Hydrodynamics codes. The point-by-point comparison of the experimental results and numerical simulations revealed advantages and disadvantages of these two methods in capturing the overall behavior and pore-scale phenomena, including residual saturations, formation of thin films, fluid bridges and various fluid trapping mechanisms.

Numerical Simulations of Three-Phase Relative Permeability in Berea Sandstone using Lattice Boltzmann Method

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ABSTRACT

Under the growing energy demand in the world, geological CO2 sequestration combined with Enhanced oil recovery (EOR) technologies is considered a promising solution for reducing carbon emissions into the atmosphere with economic benefits by recovering oil at the same time. EOR using CO2 injection into depleted oil reservoirs has great potential for both long-term and low-cost sequestration of CO2. Optimization of injection strategies to maximum CO2 storage and increase the oil recovery factors requires complicated pore scale flow information within the reservoir system of coexisting oil water and CO2 phases. In this paper, an immiscible three-phase lattice-Boltzmann model is developed to investigate the complicated flow state with interaction among water, oil and CO2 system in porous media. Two main mechanisms of oil remobilization (double-drainage and film flow) have been captured by our model. Estimation method of three-phase relative permeability depending on different initial oil saturation conditions are proposed using following procedures. First, the residual oil distributions are artificially generated by the equilibrium state, which is simulated by our two-phase LB code from random water-oil distributions with the target saturation. Second, displacement processes by injecting CO2 into the digital rock sample initialized with the generated oil and water distributions in the first step. Finally, the three-phase relative permeability are calculated from the intermediate state of three-phase distribution during the displacement process. The results indicate that relative permeability of CO2 calculated by our steady state method is insensitive to the invading fluid history and initial topology which have high impact on the drainage and imbibition process, (snap off, corner reverse filling etc.). From the results of current numerical implementation, it is suggested that a given relative permeability independent of invading fluid history may be sufficient for the large-scale reservoir simulation.

Experimental and numerical investigation of CO2 gas flow in an intermediate flow cell using a modified invasion percolation model

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ABSTRACT

We will perform invasion percolation simulations using a modified invasion percolation (MIP) model in order to understand and quantify the physics of the transition from compact flow to capillary channel flow. Our modified invasion percolation (MIP) modeling includes the validation of several modifications of the classical invasion percolation algorithm for modeling phase displacements in fractured and porous media system. The key feature of the MIP algorithm is that it accounts for the curvature of fluid-fluid interfaces across the aperture and in the plane of the fracture, and stochastic selection and invasion features for a wide range of capillary and Bond numbers (Glass et al., 2000, 2003; Ewing and Berkowitz, 1998). The MIP model will be vigorously validated against well-controlled intermediate scale 2D sandbox experimental datasets. A heterogeneous pattern was created mimicking a fluvial sedimentary deposition pattern (Glass et al., 2000). The CO2 gas injection rates varied from 0.1 ml/min to 5 ml/min and buoyancy-driven nonwetting invasion patterns were quantitatively observed at ~ millimeter scale using the light transmission system. Experimental results demonstrate that multiple pathways of gas flow was observed at the top of fine and coarse sand interface depending on the CO2 flow rate, which was caused by both viscous and capillary-gravity pulsation. Previous MIP modeling results had a good agreement with CO2 gas flow for a low flow rate case. We will further evaluate the impact of MIP parameters of Ewing and Berkowitz model. We will demonstrate that the validated MIP model can be used to develop new experimental-informed, physics-based models of the transition process, focused on representing cm-scale heterogeneity.

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Immiscible fluid displacement patterns under various reservoir conditions and their influence on geophysical properties

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ABSTRACT

The behavior of CO2 inside a reservoir in Carbon Capture and Storage (CCS) can be characterized as two-phase flow. The two-phase fluid behavior is influenced by temperature, interfacial tension, pore structure, and porous medium characteristics (e.g., wettability), which vary significantly from one reservoir to the next. Pore-scale interfacial instabilities, such as snap-off and fingering phenomena, influence the stability, injectivity, mobility, and saturation of CO2 within the reservoir. Therefore, understanding microscopic CO2 flow in porous media is crucial to estimating storage capacity, leakage risk, and storage efficiency. Furthermore, the geophysical properties (e.g., seismic velocity) influenced by CO2 flow behaviors could be useful to reveal CO2 flow patterns in the reservoir. Here we calculated fluid displacements within (1) Berea sandstone and (2) homogeneous granular pore model using two-phase lattice Boltzmann (LB) simulation, in order to characterize the influence of reservoir conditions and pore geometry upon multiphase flow. We classified the two-phase flow behavior that occurred under various conditions into three typical fluid displacement patterns on the diagram of capillary number (Ca) and viscosity ratio of the two fluids (M). The results revealed the onset of capillary fingering in natural rock at a higher Ca than the 2D homogeneous porous media, with the crossover region between typical displacement patterns much broader than in the 2D homogeneous granular model. These differences between two-phase flow in natural rock and in a homogeneous porous structure could be the result of the heterogeneity of the natural rock. By mapping the CO2 saturation on the Ca-M diagram, furthermore, we could identify the suitable environments in CCS or geofluid managements. We then calculated geophysical properties (seismic velocity and electric resistivity) of the digital rock models using numerical simulations (e.g., dynamic wave propagation simulation) in order to characterize the CO2 displacement patterns from geophysical properties. By comparing these calculated geophysical properties and experimental results (or result of geophysical monitoring), we could predict in situ CO2 behavior.

Mixing and reactive transport under unsaturated conditions: a pore scale study

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ABSTRACT

Predicting the transport of chemical species through unsaturated porous media is still an open issue. The spatial distribution of wetting (e.g., water) and non-wetting (e.g., air) clusters focuses the water flow onto narrow and complex flow paths., leaving large volumes of wetting fluid trapped in between non-wetting phase clusters. As a consequence, the dispersion and mixing of solute elements strongly depends on the saturation degree, which is in turn critical for the prediction of reactive transport processes. We study the dependence on saturation of the longitudinal dispersion coefficient and the temporal scaling properties of mixing in variably saturated porous media consisting of cylindrical grains positioned inside a Hele-Shaw cell. The medium is built using soft lithography. The joint injection of the two phases (wetting and non-wetting) provides a controlled homogeneous saturation in the medium. The simultaneous measurement of the flow velocity field, the spatial distribution of the wetting and non-wetting phases, and the tracer concentration field allows investigating the relationship between the flow field complexity induced by desaturation and dispersion/mixing properties. We analyze the temporal behavior of the mean concentration gradient and scalar dissipation rate; this behavior controls the potential for mixing-controlled chemical reactivity. While for a continuous injection under saturated conditions the mean concentration gradient decays in time according to the classical diffusive smoothing of concentration gradients, the creation of highly channelized finger structures, separated by air bubbles, in unsaturated flows induces persistently large concentration gradients that decay slowly in time [1]. We show that this effect is due to i) a drastic increase of the surface available to concentration gradients across the finger boundaries, ii) the mostly longitudinal orientation of the solute fingers, and iii) the near impossibility for these fingers to coalescence along the direction transverse to the mean flow, except at critical bottle necks formed between air clusters. These results suggest that large concentration gradients may persist over a broad range of times in unsaturated media. For hydrological systems, this would suggest a larger reactivity under unsaturated conditions, up to the scale of the largest air bubbles. For a pulse line injection we also find that desaturation induces anomalous temporal scaling of the longitudinal dispersion (super-diffusive) and scalar dissipation rate [2]. This effect is particularly relevant for upscaling reactive transport.

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Pore-Scale Flow Interactions Between Water and Supercritical CO2 in 2D Heterogeneous Micromodels at Reservoir Conditions

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ABSTRACT

Multiphase flow of water and supercritical CO2 in porous media is central to the geologic sequestration of CO2 within saline aquifers. The coupled flow dynamics of CO2 and brine in geologic media must be better understood, particularly at the pore scale, as pore-scale processes represent a critical component of accurately predicting large-scale migration of injected CO2. To this end, the pore-scale flow interactions of water and liquid/supercritical CO2 are presently being quantified in 2D heterogeneous porous micromodels at reservoir-relevant conditions (i.e., 80 bar, 20 degC), in an attempt to accurately mimics the process of CO2 injection into saline aquifers. The micromodels used in these experiments were fabricated from silicon, with the porous matrix formed from the reprint of the pore structure of real sandstone [1]. Fluorescent microscopy and the micro-PIV method are employed by seeding the water phase with fluorescent particles and tagging the CO2 phase with a fluorescent dye of a different spectral emission. Doing so allows for simultaneous measurement of the spatially-resolved instantaneous water velocity field and quantification of the instantaneous spatial configuration of both phases [2]. The initial results provide a clear picture of the flow physics during the migration of the CO2 front, the evolution of individual menisci and the growth of dendritic structures, so-called fingers [2]. During the CO2 infiltration process, CO2 suddenly breaks through the resident water, forming fingers which grow in directions both along and normal to the bulk pressure gradient, and even against the bulk pressure gradient, indicative of capillary fingering. The complex phase configuration highlights the importance of local pressure gradients in CO2 front migration. Moreover, the respective experiments are being done collaboratively with complementary numerical simulations and these experimental data will be directly compared with the simulation results, yielding valuable insight into flow processes at the pore scale in natural rock.

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Pore network modeling and experimental evaluation of nanoparticle carbonation in a shale matrix

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ABSTRACT

Shale oil/gas production in US has increased dramatically in recent years even though the environmental implications of this activity are still poorly understood. Seepage and leakage of fracturing fluids or fugitive methane emissions could impact fresh water aquifers and human health near the surface. Our lab is pioneering a technique to deploy reactive proppants during the fracturing process that can later be used to seal the fractured shale formation. The method could be used to limit the fluid conductivity of shale fractures/pores via mineral carbonation reactions that would be initiated by injecting high pressure CO2 before closing the well. Any calcium/magnesium silicate could be used and after reacting with CO2 would form precipitated calcium or magnesium carbonate and silica. This class of mineral carbonation reaction has been applied as an ex-situ method to capture CO2 from power plants. Here we explore the effect that these precipitation reactions would have on the flow properties of a packed column experiment under pressure temperatures that are representative of a shale reservoir. Then pore network modeling simulations were used to model the experiments and help optimize the conditions under which this class of carbonation reactions could be used to cement and seal fractured shale.

Column experiments were carried out under pressure and temperature conditions representative of the Marcellus Shale formation. CaSiO3 (wollastonite) was used as the representative silicate mineral. Both Scanning Electron Microscopy (SEM) images and X-ray diffraction (XRD) patterns indicate the precipitation of carbonate minerals with crystal size ranging from 1 to 5 μm, covering the shale particle surfaces. Mercury Injection Porosimetry (MIP) of the columns reveals obvious changes of the pore structures of the packed mineral samples. Permeability decreased by 50% was predicted according to the porosity change through empirical Swanson equations. In parallel, a Pore Network Modeling (PNM) framework was implemented to explore the changes in the pore structure under different scenarios. The evolution of carbonation front is shown to be controlled by pH, temperature, pressure and initial CO2/Ca2+ concentration. Both experimental and simulation results indicate that the precipitated CaCO3 in shale matrix is likely to decrease conductivity. As a result, the leakage risk in hydraulically fractured formations following hydrocarbon exploration could be controlled.

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Gas injection into water-saturated sand: comparing experiments to macroscopic invasion percolation simulations

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ABSTRACT

An understanding of gas flow is important in many subsurface systems, including those related to oil and gas recovery, geologic carbon dioxide storage, groundwater remediation and shale gas development. Upwards gas flow can occur as a network of continuous channels or as discontinuous gas bubbles, depending on the balance of viscous, gravity and capillary forces, with bubble flow occurring for slower gas flow in coarse-grained media. Macroscopic invasion percolation (macro-IP) techniques offer an alternative approach over continuum-scale modelling approaches, capable of reproducing important aspects of unstable gas flow at a low computational cost, which allows the simulation of larger domains and multiple realizations. However, there have been few studies that have compared the results of macro-IP simulations to experiments on the basis of local gas saturations. In this study, small-scale (10 cm) gas injection experiments were performed in a quasi-two-dimensional flow cell initially packed with water-saturated sand. Gas was injected slowly and local gas saturations (mm-scale) were measured using light transmission imaging techniques. The observations were directly compared to gas injection simulations performed using a macro-IP approach that included fragmentation and mobilization to reproduce gas bubble flow. Simulations were performed in both two-dimensional (thickness-averaged) and three-dimensional domains, both with and without a modification to account for viscous forces (stochastic selection). Simulations were conducted as a Monte Carlo study using multiple realizations (1000 per test condition) of the entry and terminal pressure fields. Comparisons were based on spatial moments of the observed and simulated gas distributions, as well as local gas saturation values. Results showed that two-dimensional simulations were capable of reproducing observations from think-tank experiments, and that modifications to account for viscous forces were required to match the width of injected gas distributions in finely-resolved three-dimensional simulations.

Characterisation of microstructural and physical properties changes in sand induced by biocementation using 3D x-ray synchrotron microtomography

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ABSTRACT

Soil reinforcement by the Microbial induced calcite precipitation (MICP) has received attention in recent years; due to its economic and environmental advantages to strengthen the soil against various geotechnical problems (sliding slopes, dam's internal erosion, and sand foundation liquefaction). The calcite precipitates in the voids of sand porous media in two different manners (between grains and on grains surfaces). The calcite that precipitates on grain contacts forms cement bridges, which give cohesion to the sand specimens. On the other hand, when calcite precipitates on the grains surface, it provides additional grain roughness. The influence of the biocementation process on the microstructural and physical properties changes are not clearly established. For that purpose, an experimental study has been performed to explore the effect of calcification on the microstructural and the physical properties of a series of biocemented Fontainebleau sand samples, with various cementation levels. The microstructural properties (porosity, specific surface area, volume fraction of calcite, correlation lengths) of the biocemented samples are estimated from 3D images obtained by X-ray synchrotron microtomography. In parallel, some physical properties such as the permeability and effective diffusion tensors are computed on Representative Elementary Volume extracted from the 3D images by solving specific boundary problems arising from the homogenization. All the quantities deduced from the 3D images are then compared, when it is possible, to experimental values. A good consistency is found between the experimental and the numerical results. The strong influence of the biocementation level on some physical properties such the permeability is shown and discussed.

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Comparison of experiments, lattice-Boltzmann simulations, and theory for drainage and imbibition in pore doublets

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ABSTRACT

In this work, we revisit the dynamics of immiscible displacement in pore doublets. The pore doublet consists of two channels of different cross-sectional areas that split from a single channel and then reconnect to a single channel. We conduct a series of pore doublet drainage and imbibition experiments involving oil-brine and supercritical CO2-brine and compare our results to (1) lattice-Boltzmann simulations and (2) existing theories for this relatively simple system. We show that in many cases the experiments, LB simulations, and theory are in qualitative agreement in regards to the trapping of fluids within the channels. We also measure interface velocities and pore filling times within the pore doublets in order to provide a more quantitative comparison. In our experiments, we observe wetting phase films, which the existing theories do not consider, and compare these results with LB simulations. We show that the existence of wetting phase films affects the displacement processes and trapping of fluids.

Microstructure of the Mt Simon Sandstone and its interaction with simulated reservoir brine and CO2 under reservoir pressure conditions

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ABSTRACT

Accurate descriptions of the interactions between injected carbon dioxide (CO2), sandstone matrix and synthetic brine on the micrometer and submicron scale are difficult to achieve but crucial to expanding our understanding of CO2 storage in reservoir rock. The Mount Simon sandstone with its combination of thickness, depth and overlying impermeable layers is a critical reservoir for understanding carbon sequestration's full potential. As part of the Center for Geologic Storage of CO2, this work characterizes the Mount Simon sandstone under reservoir pressures at single micron and smaller scales. Due to the heterogeneity of the Mount Simon, single micron scales frequently represent data at or below the representative elementary volume.
An Xradia Micro-CT scanner was used to image pore spaces in flow-through experiments under reservoir pressures. A beryllium containment vessel, capable of withstanding in excess of 2500psi, holds the approximately 1 cm long sample. ISCO pumps are able to deliver both brine and CO2 to the vessel under reservoir pressures and maintain them for several days, allowing for numerous scans under meta-stable conditions.

The resultant 3-D imagery of the discrete phases (matrix, brine, and CO2) are the basis for several measured geological parameters, such as porosity and capillary resistance, and for the determination of storage capacity. At the highest resolutions (approximately one micron) it is possible to directly image wetting angles, improving our understanding of them in more complex, natural settings. Binary images created from these scans which separate pore space from matrix provide fundamental data needed in numerical flow modeling techniques to better characterize the Mt. Simon sandstone, giving a more complete picture. Finally, the most recent sub-micron scale images provide additional insight on the smallest flow-paths for CO2 migration.

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Mixing in a three-phase system: re-stimulation of oil-wet reservoirs by CO2 injection

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ABSTRACT

Three-phase reservoir conditions (high-pressure/temperature) have been recreated using a microfluidics system. We show that the use of scCO2 for re-stimulation operations, such as hydraulic fracturing, in oil-wet reservoirs (e.g., limestone, chalk and shale) can enhance mixing and production. Production decreases rapidly and methods to increase efficiency or allow re-stimulation of wells are needed. In our experiments, the natural presence of brine and/or from initial production creates spatio-temporal variability in the heterogeneity of system that causes the injected scCO2 to more effectively interact-mix with trapped hydrocarbon, thereby increasing recovery. We apply volume-averaging techniques to upscale brine saturation, which allows us to analyze the complex three-phase system in the framework of well characterized two-phase systems. The upscaled three-phase system behaves like a two-phase system: greater mixing with larger non-wetting content and higher heterogeneity. The results are contrary to previous observations in water-wet systems.

Comparison of Lattice Boltzmann Simulation and Experiment of Pore-Scale Flow Interactions Between Water and Supercritical CO2 in 2D Heterogeneous Micromodels at Reservoir Conditions

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ABSTRACT

Multiphase flow of water and supercritical CO2 (scCO2) in porous media is central to the geologic sequestration of CO2 within saline aquifers. Due to the limitation and expense of experiment measurements, it is very difficult to observe the interactions between water and scCO2 in real 3D rock. Direct numerical simulation, such as the lattice Boltzmann method (LBM) simulation, can provide detailed flow information in real 3D rock core and is a promising way to study the fluids interactions in porous media. The effectiveness of such simulation is validated by comparing bulk properties with experiment data, such as the relative permeability-saturation curve. Whether local flow patterns could be correctly captured by the numerical simulation may be questioned. Therefore, comparison of the flow patterns between the direct numerical simulation and 2D porous micromodel experiment is important for the validation of numerical simulation. Previous comparisons between 2D micromodel experiment and numerical simulation were mainly performed on homogenous models. In this study, we will compare LBM simulation results with flow data obtained from 2D heterogeneous micromodel experiment under reservoir conditions. The multiphase model used in the LBM simulation is the color-fluid model due to its sharp interface and strictly immiscible property. Some new improvements of the multiphase model will be employed to reduce numerical errors and match the fluid properties.

Acknowledgements
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A discrete-domain description of multiphase flow in porous media: Rugged energy landscapes and the origin of hysteresis

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ABSTRACT

We propose a discrete-domain model to describe mesoscale (many-pore) immiscible displacements in porous media. We conceptualize the porous medium and fluid system as a set of weakly connected multistable compartments. The overall properties of the system emerge from the small-scale compartment dynamics. Our model aims at capturing the rugged energy landscape of multiphase porous media systems, emphasizing the role of metastability and local equilibria in the origin of hysteresis. Under two-phase displacements, the system behaves hysteretically, but our description does not rely on past saturations, turning points, or drainage/imbibition labels. We characterize the connection between micro-metastability and overall system behavior, and elucidate the different nature of pressure-controlled and rate-controlled immiscible displacements in porous media.

A numerical study on evolving pore distribution in granular materials

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ABSTRACT

Micro-structure of any granular geomaterials such as sand, rock etc. plays a pivotal role on the deformation behaviour as well as the pore-fluid flow properties. While the size and shape of individual grains and their packing defines the micro-structure, exact quantification of such packing is not trivial and thus as an indirect measure macroscopic porosity often used. The variation in porosity during the deformation process indicates rearrangement of grains and formation of new packing by means of dilation and compaction. Nevertheless, porosity only serves as a global measure. Pore volume distribution on the contrary provides much richer information regarding the micro-structure. It is one of the key ingredients for various flow related geotechnical problems such as erosion, piping, and infiltration as well as filter design (Raut & Indraratna, 2008). Even the nature of soil moisture interaction which is crucial for unsaturated soils, depends on the distribution of pore spaces (Li & Zhang, 2007).
Despite advanced methodologies (e.g. imaging technique or numerical methods), evolution of pore volume distribution during shear deformation has never been explored systematically. In the present study evolution characteristics of pore volume distribution is theoretically captured at various stages of deformation for numerically simulated granular assemblies generated through Discrete Element Modelling (DEM). A simplified algorithm based on the propositions of Gao et al. (2012) is used for the estimation of pore volume distribution. It is well known that depending on the initial state of any granular specimen, either loose or dense, inter-granular pore spaces undergo contraction or dilation during shear deformation and finally converge towards a unique critical porosity. Present study shows that pore volume distribution also exhibits similar trend under shearing and finally converges towards a critical distribution (see Fig). Such observations are utilized further to demonstrate the effects of pore volume evolution on the flow of fluid through granular filters as well as for the estimation of energy dissipation during inelastic deformation process.

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A Thermo-Hydro-Mechanical Model of Freezing in Saturated Soils for Geothermal Applications

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ABSTRACT

In shallow geothermal applications, freezing processes caused by continuous heat extraction in cold regions can affect the heat pump's performance or damage the borehole heat exchangers (BHE). This phenomenon dramatically influences the subsurface soil temperature distribution, groundwater path and can in extreme cases damage a building's foundation. On the thermal aspect, the influence of soil freezing on BHE efficiency has already been studied in Zheng et al. But to quantitatively evaluate the integrated impact of freezing on different physical aspects simultaneously, a fully coupled thermo-hydro-mechanical freezing model is established and coupled to a numerical model of a shallow geothermal heat pump system.

The THM model is based on the Theory of Porous Media. The entropy inequality is utilized to derive the thermodynamically consistent - constitutive laws to supplement the macroscopic balance equations. We introduce both kinetic and equilibrium approaches for ice formation in the model. The specific relations of the evolution or equilibrium equations characterizing the freezing process can be formulated to account for typical features observed during phase changes occurring in porous media. To accommodate for large volume dilatations induced by ice formation, a finite strain approach is chosen. While the THM model itself can describe phase changes in porous media in a general way, the coupling to the numerical BHE model makes it especially suitable for shallow geothermal applications.

The numerical model will be implemented into the open source framework OpenGeoSys based on the finite element method. The coupled processes are solved monolithically and the non-linearity is solved by an incremental-iterative Newton-Raphson strategy. Verification will be performed based on common benchmark problems.

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Investigation on the physical mechanism of enhanced coal bed methane recovery with continues vibration

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ABSTRACT

The continuous pulse shock and vibration has been applied as an effective physical method for enhanced coal bed methane (CBM) recovery as it can changes the occurrence state of gas in coal and cause coal seam permeability to be significantly improved. Considering that stress change, CBM migration, pores and fractures structure evolution, and matrix deformation proceed simultaneously, and has interaction obviously, these processes were researched. a coupled numerical model of vibration enhanced CBM recovery, which regards all the aspects of interaction, is established based on the internal pore and fracture structures. The model is evaluated using data from a number of experimental tests published in the literature. The coupled flow and transport process of methane in coal seams under vibration by numerical simulating based on the proposed model is discussed. The model can reflect the evolution trends of permeability in vibration and other stress conditions. Furthermore, the interaction between coal fracture and coal matrix, its law of influence on permeability of coal rock, and the law of interaction between effective stress and permeability of CBM are investigated.

Evolving Porous Media mechanism, experiments and application in resources and energy exploitation

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ABSTRACT

A wide range of solid media gradually evolve into porous media containing a large number of pores, and sometimes voids and fractures, after a single or several coupled physical and chemical actions. This is a very common phenomenon in nature, where permeability increases with porosity and less developed fractured porous media transform to highly developed media. In our studies, the evolution phenomena and mechanism of porous media were analyzed according to the driving factors, i.e., external force, heat, seepage, coupled chemical reaction and seepage, coupled chemical reaction and heat flow. According to the evolution mechanism, the evolution can be categorized as three types?ie natural evolution, artificial evolution, and natural–artificial evolution.
This paper introduces in detail the evolution mechanism of three types of porous media, the role of evolution and evolution process and results in engineering meaning.
evolution process in porous media is quantitative characterized with relationship of evolution of porosity and permeability of porous medium.
This paper introduces a few industrial applications with our apply by evolution mechanism of the porous medium?include ?the hot dry rock geothermal development, glauberite ore deposit mining, mining oil and gas with lignite in situ pyrolytic.
1) Introduced the HDR geothermal resource development in the study, from room temperature to 600 ? and high pressure under the action of 5000-6000 m deep strata stress, experimental study on granite pores and fissures of the occurrence and development, with means: acoustic emission detection, microscopic CT mesoscopic observational , along with progress of permeability change. Deep of high quality hot dry rock geothermal energy development and improvement of technical solutions.
2) Introduced the three type of Chinese origin of lignite coal sample, from room temperature to 600 ?,the evolution of the pore and fissure, evolution process with lignite pyrolysis gas liquid product components and output of the corresponding permeability changing with the temperature. Introduces the in situ pyrolytic lignite mining of oil and gas.
3) sodium glauberite ore is a kind of important mineral resources, it is the main component of sodium sulfate, calcium sulfate, among them the content of sodium sulfate is 30%, its dissolving process, of glauberite ore porosity increased gradually, the pore connectivity increasing. Dissolve in chemical reaction conditions are introduced in detail in this paper, the porous media evolution of glauberite ore mechanism , evolution process and the evolution results for mining the significance of sodium sulfate and calcium glauber's salt deposit in situ mining technology application.

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The micron-size pore evolution law of oil shale under different temperature

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ABSTRACT

Nano-scale pore is the main place of fluid absorbed, micron-size pore is the main channel of fluid flow. The micron-size pore evolution law of oil shale under different temperature conditions were observed and analyzed based on high precision micro-CT technology. The achieved results show 300? is the abrupt change point of the oil shale micron-size pore structure change. When the temperature is below 300?, oil shale micron-size pore structure change is not obvious, and from 300? to 500?, the pore number and average pore diameter and porosity are the rapid growth in sync, among them, the average pore diameter increased from 1.52?m to 1.72?m and the porosity increased from 8% to 12%. The main reason is the pyrolysis of organic matter in oil shale after generating a large number of oil and gas from 300? to 500?, it make the place occupied by the oil shale organic matter evolved out a large number of new pores, these new pores can be used as a bridge to connect the original pores. Thus causing the number of pores in diameter greater than 1.50?m is increased, while the diameter of less than 1.50?m pore number is reduced due to the join of these pores, which fundamentally improved the percolation ability of oil shale.

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Pyrolysis induced cracking in coal

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ABSTRACT

In the projects of coal underground gasification, heat-injection enhanced coalbed methane recovery, coal is in both in-situ stresses field and temperature field. Pyrolysis will take place in coal while temperature increases from room temperature to 600 centigrade and the structure also changes. We use high-resolution computerized tomography technology to observe mesostructure evolution of lignite and gas coal at elevated temperature. At low temperature phase (<300?), quantities of cracks generate induced by the release of water component and free gas in coal matrix, and a great number of pores and fissures induced by pyrolysis of coal emerge at high temperature phase (>300?). In this paper, we name this phenomenon that such organic-matter-rich rock like coal generates damage due to pyrolysis effect as pyrolytic cracking which is definitely different from thermal cracking in inorganic rock such as granite, sandstone, et.al. Compared with thermal cracking, it is unique for pyrolytic cracking that involving damage mechanism, initial damage location and crack morphology. Figures 1 and 2 show morphology of pyrolytic cracking in lignite and gas coal. New cracks induced by the release of water component and free gas at temperature below 300? is gracile crack which is formed not only at the boundary of two hard minerals but also widely in the organic matter. And the morphology of new cracks induced by pyrolysis at temperature over 300? is circular and elliptical pores which is formed only in the organic matter.

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Influence of the Stress Sensitivity on Microcosmic Pore Structure and Fluid Flow in Porous Media

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ABSTRACT

At present, large quantities of experiments related to stress sensitivities on macro-scale have been studied. Pore structure is complicated, especially the unconventional reservoirs like tight sandstone, so stress sensitivity would have a great influence on changing the pore space. It is of great significance for development and enhancing the EOR to study the stress sensitivity systematically on pore scale. In this paper, based on CT scanning technology which could capture the pore space characters of the real core, combing the technology of digital core and pore network model, the relationship between the effective stress change and the pore structure is obtained. First, the theory and method of constructing the digital core and extracting the pore network model according to CT scanning is introduced. 3D core image could be got after CT scanning, and digital core is established after filtering and segmentation. The rock structure characters could be got when analyzing the geometry-topology structure of the pore network model extracted, and the fluid flow analysis could be got after flow numerical simulation. Second, the method of stress sensitivity experiment and analysis is built on the basis of manmade sandstone. Stress sensitivity experiments are carried out in the carbon fiber core holder, and the core is scanned under a series of pressures. As well as this, digital cores and pore network models under a series of pressures could be obtained, and the corresponding pore structure characters and fluid flow laws could be analyzed. Third, this method could be used in the meso-high permeability sandstone and tight sandstone. The stress sensitivities of these sandstones are achieved and compared. In this paper, one comparative integral stress sensitivity evaluation method is formed, which would have the value of practical application on enhancing the oil recovery.

Research on distribution rule of landfill settlement with considering filling process

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ABSTRACT

With the improvement of living standards, it is very important to deal with the waste in cities. Land filling is one of the most economical and efficient ways to treat Municipal Solid Waste (MSW) in our country on the long section of times. Because of the waste degradation and stabilization process, landfill will have a huge settlement in a very long period of time, and the numbers of the landfill layers have influence on the settlement of the landfill. The huge settlement will impact refuse of land and will break the protection system of landfill. In addition, it will seriously affect the management and operation of landfill site, then threatening the surrounding environment and personal safety. Therefore, the settlement of MSW landfill is a principal geotechnical engineering problem of sanitary landfilling. According to filling process of municipal solid waste, the landfill model was built. Combined with specific case study the distribution rule of the landfill settlement was calculated when considering filling process and not considering. Meanwhile, change rules of settlement displacement were obtained along with the depths of landfill. It was also analyzed that the maximum settlement changes with the number of landfill layers, then the curve of maximum settlement and the number of landfill layers was obtained. Studies have shown that: when considering filling process, the largest landfill settlement occurred in the middle of the landfill within a 40 m-60 m depth range, which was about 14.60 m. When filling process was not considered, the maximum landfill settlement occurred at the top of landfill, approximately 22.63 m. Above all, the former produced a small settlement than the latter. At the same depth of the landfill, the settlement in upstream was slightly larger than the downstream. With the increased of the landfill layer the maximum settlement decreased, and the rate of maximum settlement decreased gradually.

The Application of Finite Element Modeling for Multiple-fracture Horizontal Wells in Tight Oil Reservoirs

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ABSTRACT

Multiple-fracture horizontal wells (MFHWs) have become the most effective technology for exploiting in low permeability unconventional reservoirs, such as shale gas reservoirs, tight oil & gas reservoirs. Because MFHWs incorporated with massive hydraulic fracturing, the theory and application are challenges compared with conventional reservoirs. Accordingly, a novel mathematical model of MFHWs based on discrete-fracture model in which the hydraulic fractures are discretized as 2D entities is developed in this paper, the reservoir geometry is discretized using tetrahedron elements and triangular elements for the hydraulic fractures. Then, solution of the problem is obtained by Galerkin finite element method in this work. The methodology can greatly reduce the number of meshing grids, computational complexity, while the reasonable computational accuracy and efficiency is maintained. The approach can be used to history match and forecast well performance (like production, bottom hole pressure, average formation pressure, et al) from MFHWs under the inner condition of constant bottom hole pressure, constant production rate, intermittent production, or even more complex production rules, at the same time, the reservoir can be arbitrary shaped with constant pressure, closed, or mixed outer boundary condition. Furthermore, rate and pressure transient analysis of MFHWs in tight oil reservoirs are investigated based on the model that have been developed. Finally, two examples of field data are matched to support the approach in this paper.

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Research of oil shale pore structure evolution with temperature

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ABSTRACT

It’s most important to understand the pore structure evolution under temperature while in-situ mining method was used to recovery the oil and gas in oil shale. Oil shale is a kind of shale rock but contains kerogen which can be recovered by heating. While oil shale was heated, the kerogen in it will change state from solid to liquid or even to gas while the temperature is high enough. During the in-situ recovery of oil shale, all the produced shale oil and oil gas, both in liquid state or gas state, need to leakage from different pores to big fractures and then to product wells. In this process, the heat will not only affect the deformation of rock itself, but also make the state change of kerogen. This will make the pore structures evolution in oil shale more complex. In order to find out the dynamic change regularity of pore structure evolution, we applied Mercury Intrusion Porosimetry (MIP) method to test the oil shale pore structure evolution under different temperature. From the results we can see: 1) the medium pore diameter and average pore diameter has the same change regularity as the temperature increase. Both of them increased as the temperature increase; 2) the porosity and the effective porosity almost have the same change regularity when the temperature is below 500, when the temperature is high than 500, the porosity is still increase with temperature while the effective porosity begin to; meanwhile the permeability is continuously increasing with temperature increase. 3) In order to research the change law of pores with different diameter the pores in oil shale are divided into four groups based on the pore diameter, one can see then when the temperature is below 400, as temperature increase, the percentage of different size pores almost have no change; but when the temperature is high than 400, the macro pores have a sudden decrease, and the micro pores almost disappeared, but at the same time, the meso-pores has a great increment and begin to be the main part to form the seepage channel

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Preferential Adsorption of Volatile Hydrocarbons over High Surface Area Chalcogels KMBiTe3 (M = Cr, Zn, Fe)

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ABSTRACT

Separation of hydrocarbons with similar boiling boints is difficult to achieve using conventional methods such as fractional distillation.1 Different technologies have been developed, e.g., adsorptive separation using ionic liquids can enhance the separation process, but the cost of ionic liquids prevents commercial applications.2 Polymeric membranes have also been employed for volatile hydrocarbon separations, but they require harsh operation conditions Such as: high temperature.3 Currently, several porous materials, e.g. zeolites, silica gels or activated carbons are used as adsorbents. Among them, metal chalcogenide aerogels area new type of porous materials which can be used as selective adsorbents for volatile hydrocarbons.4 In this study, three new chalcogels, KCrBiTe3, KZnBiTe3, KFeBiTe3, were synthesized and evaluated as adsorbents for a number of hydrocarbons and gases. BET surface area measurements after supercritical drying of the chalcogels is produced porous materials with a surface area of 230, 450 and 514 m2/g, respectively. These chalcogels show preferential adsorption of toluene vapor over cyclohexane vapor. High adsorption selectivities for CO2 over CH4 and H2 were calculated from single-component adsorption data.

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TOWARDS A MULTIPHYSICAL MODEL FOR SIGNALING IN NERVES AND BIOMEMBRANES

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ABSTRACT

The biological membrane is the medium for the transport processes and cell signaling and it acts as a structural barrier to the cells. The most abundant component of the membrane is a class of small molecules called lipids, which serve as a sheet into which other, larger units such as proteins are embedded. Furthermore, bio-membranes maintain non-equilibrium ion distributions across themselves, which create potential differences between the interior of the cell and the environment (the interior being more negative). In neurons, the trans-membrane potentials are essential for the generation and propagation of the nerve pulse. In this respect, the lipid matrix is believed to provide electrical insulation to the cell, all the action being attributed to specific protein channels. With this assumption, the electrical phenomenon in the neuron's membrane is represented as an electrical circuit [1] in which the lipid bilayer acts as a capacitor and the protein channels provide a passage for the ionic currents. The current Im through the membrane is given by:

where Cm is the membrane capacitance, V is voltage, gi (i being the index for a particular ion) is the conductance, Ei are the Nernst potentials of different ions. The capacitive term Cm in the above equation is derived in the assumption of constant capacitance, which however is not constant in physiological conditions as the lipids undergo phase transitions [2].

The melting transitions of lipid matrix involves severe structural changes in the membrane's area and thickness [2] and can dramatically affect the capacitance value [3]. In addition, the voltage dependence of the capacitance of lipid bilayers and biological membranes is a known phenomenon that has been widely investigated in the past [4], [5]. Nevertheless, all these considerations are generally neglected in the interpretation of electrophysiological experiments and models.

To this end, firstly we look into the membrane electrostatics to understand the origin of transmembrane potential. In the lipid matrix approximately 10-40% of the naturally occurring lipids carry a charge - usually one or two negative charges. The rest of the lipids are neutral or zwitterionic. Such zwitterionic lipids in contact with water dipoles contribute to the surface and dipole potential of the membrane. This is due to the dipole-dipole interactions between them which affect the permittivity. To study the role of zwitterionic lipids in the transmembrane potential, we modeled a zwitterionic lipid layer in contact with pure water at saturation regime with spatially varying permittivity [6]. Then the model is modified for the presence of salt ions in the medium, anions in the lipid layers in the Poisson-Boltzmann (PB) framework. To study the capacitive effects of membranes, the model is also extended accordingly.

In this contribution, firstly we present the need for a predictive multiphysical model of signaling in nerves and bio-membranes for the biomedical applications. Secondly, our approach to develop such a model through the above explained Modified-Poisson-Boltzmann (MPB) framework for the lipid layers. Finally, the effects of electro-mechanical coupling of nerve pulse phenomena based on Heimburg-Jackson theory will be explained.

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Biochemical and electrical signaling in cells on multiple scales

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ABSTRACT

In biology electrical and biochemical signals control cellular responses on a multitude of scales. Changes in local ion concentrations, following e.g. an electrical impulse, can modify the molecular conformation or binding profile of membrane embedded receptors. These changes in ion concentration can also trigger propagating electrical and biochemical signals on the larger cellular or network level. Changes in the cellular architecture then again can change how larger clusters of cells interact and process information. This exemplifies the complexity of biological signaling, organized into multiple scales. While each scale in and of itself can be stunningly complex, their vertical integration into a multi-scale machinery is the ultimate biological feat to deal with the vast amount of tasks involved in development, learning and cell survival.
In this talk we will introduce models and numerical methods for combined molecular dynamics and continuum scale simulations moving towards a multi-scale framework. The presented methods will include discretization methods for complex biological geometries, error estimation, and a coupling formalism for multi-scale simulations. Examples from neuroscience will be used to address research topics that include changes on the molecular scale, e.g. membrane-located channels or receptors, which ultimately influence the functional scale, i.e. the cellular or network level. Ultra-resolution models and methods, in which the detailed cellular and intra-cellular architecture is represented accurately in three-dimensional simulations, will be discussed using the Poisson-Nernst-Planck equations, one of the most accurate physical descriptions of current flow within electrochemistry.

A New Approach to Modeling the Skin's Polar Pathway

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ABSTRACT

The outermost, stratum corneum (SC) layer of human skin presents a formidable barrier to water loss, as well as to the ingress of xenobiotics that come in contact with the skin. It is a compact matrix of dense, keratinized cells embedded in a highly structured lipid matrix. For lipophilic permeants, the lipids are strongly size-selective; for hydrophilic permeants, they are essentially impermeable to all but the smallest solutes. Yet the SC leaks charged and other highly polar compounds at a rate many times larger than a single phospholipid bilayer. The leakage pathway is size selective with a hindrance factor consistent with cylindrical pores having radii between 16 and 32 Å.
The most cited model of this leakage pathway envisions it as a rectangular network of micropores associated with the lipid head groups.1 However, the SC lipids lack the polarity to hydrate to the same extent as phospholipids. Others have proposed an appendageal transport model with micropores associated with the epithelial lining of the skin appendages.2 However, this model focused on electrical properties and was silent on mass transport. We have developed and calibrated a mass transport model for SC consistent with this picture. The numerical solution consists of a finite difference approach to the lipid-continuous SC combined with a pseudo steady-state solution for the pores. This problem is solved within the context of the Crank-Nicolson method with a rotated band-diagonal matrix. We welcome suggestions as to other approaches to solve this problem.

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How much porous are biological membranes for drugs? Computational perspective

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ABSTRACT

Biological membranes form important barriers against the entrance of drugs or other xenobiotics either into the cell or into the human body. Theoretical estimation of the permeability of the drugs through the membranes is therefore important for the evaluation of their biological fate within the organism. While most drugs permeate biological membranes by passive permeation, some drugs are able to use specific transport and channel proteins. In both cases, the molecule has to "dig through" the membrane via route paved by instantaneous pores and cavities which forms in the drug vicinity upon its presence. Passive permeability of the drugs through this instantaneous porous pathway across the membrane is driven by its concentration gradient. Molecular dynamics (MD) simulations can be used in order to study passive permeation atomistically, but also to assess the drug's affinity towards the membrane. The major tool for such evaluation is a free energy profile along a normal axis to the membrane, which shows the affinity as well as penetration resistance for any given drug-membrane pair. We will discuss not only the methodology for free energy profile calculation in atomistic resolution, but also the effect of the membrane composition (DOPC as a cell-like membrane vs ceramide NS as a model of skin membrane) on the drug partitioning and penetration in comparison to experimental data.
In the case of porous membrane proteins, the situation is even more complicated by the much larger heterogeneity of the chemical environment within the pore. Each amino acid has distinct physicochemical properties such as size or hydrophobicity and therefore each pore has different properties as well. In order to analyse void spaces in proteins, we have developed program MOLE 2.0, which can be used to detect and analyse channels and pores of various sizes within any atomistic structure. In the case of proteins, it also gives additional information about amino acids lining the pore with detailed properties of the channel. This tool can be also assessed as MOLEonline 2.0 webservice at http://mole.upol.cz. We will show how this analysis can be used in order to study pores in membrane proteins to gain insight to their specificity and mode of action.
Overall, atomistic simulation and analysis are useful tools to gain detailed view of the biological membranes and instantaneous pores within them which can be used as an input for multiscale studies of transport properties in those systems.

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Microscopic Diffusion Model and Particle-Based Computer Simulations of Stratum Corneum Permeability

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ABSTRACT

Transient diffusion models of molecular transport through the stratum corneum (SC, barrier) layer of skin are essential tools in predicting permeation of topically applied and transdermally delivered drugs, and assessing risks associated with chemical exposures. The key to reliability of such models is a firm basis of the average diffusion and partition coefficients appearing therein in a realistic mechanistic description of the microscopic diffusion processes occurring within lipid and cornoecyte constituents of the tissue, and robust procedures to estimate the values of numerous microscopic input parameters. This talk describes a significant set of developments on various components of the microscopic picture that together produce a substantial advance upon the current generation of SC permeability models.

First, a more comprehensive analysis of SC lipid/water partition coefficients K^{lip} yields more accurate and broadly based estimates of this parameter. Second, we explicitly account for the strongly anisotropic nature of molecular diffusion within the lipid phase, quantified by a diffusivity D^{lip} = i_yi_y D^{lip,_|_} + (I – i_yi_y) D^{lip,||} where i_y denotes the unit vector pointing in the transverse (perpendicular, transdermal) direction. This essential attribute of the SC lipid phase, not considered in most SC permeability models to date, strongly affects the microscopic dynamics of diffusion. Third, a versatile, particle-based diffusion velocity method (DVM) is developed for computational simulation of the unit-cell diffusion problem in more literal geometrical representations of the microstructure. The outcome is a homogenization of all the microscopic input parameters into the tissue-average SC diffusivity D^{SC}.

Overall model results for D^{SC,_|_} are calibrated against an extensive database on hydrated SC permeability to deduce the microscopic diffusion coefficient D^{lip,_|_} for transverse (perpendicular) passage through the SC lipid phase. The tissue-average diffusivity D^{SC}=i_yi_y D^{SC,_|_} + (I – i_yi_y) D^{SC,||} comes out to be significantly anisotropic in consequence of anisotropy of both the microscopic geometry and D^{lip}. In contrast to an aggregate outcome like D^{SC,_|_} influenced by multiple microscopic mechanisms, the microscopic parameter D^{lip,_|_} exhibits a strong and understandable trend with permeant molecular weight, and can be correlated and predicted on this basis. This procedure ultimately results in a definitive upgrade of the current state of the art in predicting D^{lip,_|_} and thence D^{SC,_|_}. Also demonstrated is the ability of the model to translate skin permeability data for fully hydrated skin (the necessary state for in vitro experiments) into rational predictions for the partially hydrated state characteristic of skin in vivo.

Furthermore, the model yields predictions of D^{SC,||}, the average diffusivity for motion parallel to the plane of the SC. This parameter is crucial to quantifying the lateral spread of permeant molecules radially outward from a drug patch as they penetrate the SC.

Finally, we report on progress on a new hydrodynamic theory of hindered diffusion that is intended to model solute diffusion within more realistic representations of the keratin fiber ultrastructure inside corneocytes. Combining slender body theory and computational elements, the model sheds light on the corneocyte-phase diffusivity D^{cor}, the magnitude of which has seen controversy in the literature.

Numerical Modelling and Simulation of Systems from Biosciences

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ABSTRACT

Biological systems are distinguished by their enormous complexity and variability. That is why mathematical modelling and computational simulation of those systems is very difficult, in particular thinking of detailed models which are based on first principles. The difficulties start with geometric modelling which needs to extract basic structures from highly complex and variable phenotypes, on the other hand also has to take the statistic variability into account. Moreover, the models of the processes running on these geometries are not yet well established, since these are equally complex and often couple many scales in space and time. Thus, simulating such systems always means to put the whole frame to test, from modelling to the numerical methods and software tools used for simulation. These need to be advanced in connection with validating simulation results by comparing them to experiments.

To treat problems of this complexity, novel mathematical models, methods and software tools are necessary. In recent years, such models, numerical methods and tools have been developed, allowing to attack these problems. One of these tools is the new simulation system UG4. In the talk, we show several application examples from biology, in particular modeling the barrier property of human skin and signal processing in neurons.

Continuum-mechanical modelling and simulation of metastases growth processes within brain tissue

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ABSTRACT

A severe step in carcinogenesis is the invasion of tumour cells into the blood-vessel system resulting in metastases growth in the extra-vascular space of distant organs. In the specific case of lung cancer, tumour cells pass the blood-brain barrier to enter the brain tissue. Then, the extravasated tumour cells migrate inside the invaded tissue, form metastases and finally compromise the functionality of the affected organ due to growth processes. In general, the proliferation of the metastases is based on the available nutrient supply. To overcome a nutrient limitation, the metastases induce blood-vessel growth (angiogenesis) and form large vascularised metastases. A promising treatment of the metastases is a pressure-driven infusion of a therapeutic agent into the interstitial fluid. Besides experiments and patient studies, numerical investigations aim to improve the understanding of metastatic processes and its treatment options.
Therefore, a continuum-mechanical model of metastases growth and atrophy is presented in the framework of the Theory of Porous Media (TPM) [1]. Therein, mutually interacting components of the tissue aggregate on the microscale are superimposed based on a volumetric homogenisation of a representative elementary volume (REV). In this regard, a macroscopic model of a porous liquid-saturated solid arises. The elastic solid skeleton is perfused by two immiscible pore liquids, namely the interstitial fluid and the blood [2]. Moreover, the pore liquids are described as a real mixture of miscible components. In particular, tumour cells migrate and proliferate in the solvent of the interstitial fluid. Their growth is related to dissolved nutrients, whereas the infused therapeutic solution induces cell death (apoptosis). Furthermore, the blood consists of tumour cells embedded in the blood plasma. The extravasation, growth, angiogenesis and apoptosis are characterised by distinct mass exchange processes of the constituents in a closed-system approach of the overall aggregate.
In terms of governing equations, the model is based on the overall momentum balance, the volume balances of the pore liquids and the concentration balance of their components [3]. Consequently, the primary variables are the solid deformation, the pore pressures of the liquids and the concentrations of the solved components.
For the numerical implementation, the coupled partial differential equations are solved monolithically using the inhouse finite-element package PANDAS. Therefore, the model is discretised in space by the finite-element method (FEM) and in time by an implicit time-integration scheme. The presented numerical examples show the feasibility of the model and allow the simulation of metastases growth based on in-vitro multicellular tumour spheroids experiments.

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Skin heterogeneities and numerical simulation: A case study on accuracy requirements

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ABSTRACT

Transport processes in the skin are nowadays increasingly studied using in-silico methods. Since skin is a highly heterogeneous tissue, most approaches utilize a micro-scale model with cellular and sub-cellular resolution in order to determine the rate limiting factors correctly.

These microscopic models are typically formulated as diffusion problems that are solved on artificial, idealized geometries. This allows (i) comprising the basic relationship between morphology and function and (ii) integrating space-dependent bio-physical properties, such as partition or diffusion coefficients. State of the art models are formulated in three spatial dimensions for both the stratum corneum, as well as for the epidermis [1, 2].

In this study, we address the question, to what extent compartmental representations of the tissue are admissible, especially when heterogeneities are present in the model. To that end we investigate different configurations for the stratum corneum, its lipid bilayers, the cornified envelope, and for the epidermis. We compare homogenized and non-homogenized solutions and highlight potential pitfalls.

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Methods for simulating biochemical and electrical signals in cells on multiple scales

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ABSTRACT

In biology electrical and biochemical signals control cellular responses on a multitude of scales. Changes in local ion concentrations, following e.g. an electrical impulse, can modify the molecular conformation or binding profile of membrane embedded receptors. These changes in ion concentration can also trigger propagating electrical and biochemical signals on the larger cellular or network level. Changes in the cellular architecture then again can change how larger clusters of cells interact and process information. This exemplifies the complexity of biological signaling, organized into multiple scales. While each scale in and of itself can be stunningly complex, their vertical integration into a multi-scale machinery is the ultimate biological feat to deal with the vast amount of tasks involved in development, learning and cell survival.
This poster will introduce models and numerical methods for combined molecular dynamics and continuum scale simulations moving towards a multi-scale framework. The presented methods will include discretization methods for complex biological geometries, error estimation, and a coupling formalism for multi-scale simulations.

Size and Charge Dependence of Ion Transport in Human Nail Plate

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ABSTRACT

The electrical properties of human nail plate are poorly characterized, yet are a key determinate of the potential to treat nail diseases such as onychomycosis using iontophoresis. In order to address this deficiency, molar conductivities of 17 electrolytes comprising 12 ionic species were determined in hydrated human nail plate in vitro. Cation transport numbers across the nail for 11 of these electrolytes were determined by the electromotive force method. Effective ionic mobilities and diffusivities at infinite dilution for all ionic species were determined by regression analysis. The ratios of diffusivities in nail to those in solution were found to correlate inversely with the hydrodynamic radii of the ions according to a power law relationship having an exponent of -1.75 +/- 0.27, a substantially steeper size dependence than observed for similar experiments in skin. Effective diffusivities of cations in nail were three-fold higher than those of comparably sized anions. These results reflect the strong size and charge selectivity of the nail plate for ionic conduction and diffusion. The analysis implies that efficient transungual iontophoretic delivery of ionized drugs having radii upwards of 5 Å (approximately MW ? 340 Da) will require chemical or mechanical alteration of the nail plate.

Disrupting bacteria accumulation in heterogeneous flow structures by chemotaxis

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ABSTRACT

Subsurface bacteria influence the environmental dynamics by controlling the complex bio-geo-chemical reactions driving many important processes (such as geothermal, EOR, or bioremediation). The large-scale consequences result from the microscale interactions occurring within the subsurface heterogeneous host medium. At these microscopic scales, the subsurface environment is very heterogeneous, and both reactants and microbes experience a huge heterogeneity of chemical and physical gradients. Using microscopy and microfluidics we assess the relationship between the heterogeneous flow within a simplified analogous porous medium and the characteristic microorganism resident time and transport properties within the host medium.

Dynamics of biofilm development in porous media: bioclogging, preferential flow pathways and anomalous dispersion

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ABSTRACT

Biofilms are sessile communities of microorganisms held together by an extracellular polymeric substance that enables surface colonization. In porous media (e.g. soils, trickling filters, catheters or at the surface of membranes) biofilm growth has been shown to affect the hydrodynamics in a complex fashion at the pore-scale by either inducing preferential flow pathways and anomalous transport (Seymour, Gage et al. 2004) or clogging of individual pores (Drescher, Shen et al. 2013). These phenomena are a direct consequence of microbial growth and metabolism, mass transfer processes and complex flow fields possibly exhibiting three-dimensional features (Guglielmini, Rusconi et al. 2011). Nevertheless, the dynamics of local bacterial attachment and biofilm development, the effect of biofilms on pore networks and how bioclogging influences flow and mass transport processes is not completely understood.

This work experimentally investigates the interplay between flow, pore structure and biofilm growth in porous media. We use two spatially compatible imaging techniques to determine a) the flow and b) the distribution of biofilm in a porous medium. Three-dimensional millimodels (4x4x1.5 cm3) are packed with a transparent porous medium and a glucose solution of matching optical refractive index. The models are inoculated with planktonic wildtype bacteria and biofilm cultivated for 60 h under a constant flow and nutrient conditions. The flow in the increasingly bioclogged medium is quantified at high spatio-temporal resolution every 12 h with 3D particle tracking velocimetry (3D-PTV). The three-dimensional spatial distribution of the biofilm within the pore space is assessed by imaging the model with X-Ray microtomography priorly to inoculation and after 60 h of culturing.

In terms of changes in flow, we observed that the more bioclogging occurs, the more the flow tends to be channelized along preferential flow pathways. Therefore, the variance of longitudinal Lagrangian velocities increases with bioclogging, indicating an increase in intermittent behavior. de Anna, Le Borgne et al. (2013) linked flow intermittency with persistent anomalous dispersion, a similar observation can be made here, as the increase in intermittency observed can be linked with earlier arrival times and stronger tails of experimental breakthrough curves of passive tracers. In terms of the changes in pore structure, we observed that key features of the effective pore network change upon biofilm growth. Specific changes are observed for arc lengths, pore sizes, node degree, which are originally relatively uniformly distributed for prior to clogging, but exhibit completely different statistics at the most clogged time point. Ongoing analysis is focused on a) making the link between the network characteristics and the anomalous dispersion, and b) identifying features of channels that are more prone to be clogged or to become preferential.

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Localisation of bacteria in a Poiseuille flow

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ABSTRACT

We report experiments of transport of bacteria in a long capillay tube of small diameter. For passive particles or dead bacteria, we observed that the particles are equally distributed in the section of the tube. For living bacteria, the situation is very different. We observe en overconcentration of the bacteria in the vicinity of the surface. The density first decrease with the flow, but for shear rate above 5 Hertz, we then found that the population increases reaching values well above the density of bacteria in absence of flow. The characteristic time of the phenomena are finally introduced to explain the different bahavior observed.

Coupled transport and population growth of Pseudomonas putida bacteria in the vicinity of a toluene source plume in a saturated sand-packed two-dimensional microcosm

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ABSTRACT

The transport of microorganisms through the saturated porous matrix of soil is critical to the successful implementation of bioremediation in polluted groundwater systems. Motile bacteria that are self-propelled are able to swim independently of the groundwater flow and thereby enhance their accessibility to the hydrocarbon pollutants which they chemically transform and use as carbon and energy sources. Access to the hydrocarbons, thus provides a competitive advantage and increases the growth rate of the motile bacterial population.

A two-dimensional rectangular-shaped microcosm packed with quartz sand (1, 3) was used to study the transport and population growth of bacteria within a saturated model aquifer system (see Figure 1). Artificial groundwater was pumped through the microcosm at a rate of 1.1 m/day. A plume of toluene dissolved in the aqueous phase was created by continuous injection into the microcosm. Species of Pseudomonas putida F1, either wild-type (WT) or a genetic mutant (TodX knockout) that lacked a mechanism to transport toluene across the outer cell membrane (2), were injected along with a conservative tracer in a port several centimeters either above or below the toluene. As the injectates traversed the one-meter length of the microcosm, samples were collected from a dozen effluent ports to determine vertical concentration distributions for the bacteria and tracers.

The vertical distribution of PpF1 in the effluent from the microcosm was characterized in terms of the center of mass, variance and skewness as derived from a moment analysis. The percent recovery was also recorded to indicate population growth. These results are summarized in Table 1. These characteristics were then compared to the mutant strain PpF1 (TodX knockout). The ability to take up toluene into the cell resulted in significantly greater population growth of the WT as compared to the mutant. It should be noted that because PpF1 has a density that is greater than water, the center of mass of the bacterial distribution tended to migrate downward by about one centimeter over the 18-hour timeframe of the experiment. Regardless of this, PpF1 mutant injections above the toluene plume which had greater exposure to the toluene still showed less population growth than WT which was injected below the plume. Comparisons for low and high toluene source concentrations indicated increased population growth of PpF1 at the higher toluene concentration except for the WT in Study 2. The results for bacterial injections oriented either above or below the toluene plume are also presented in Table 1. Comparing the percent recovery of WT to mutant across Study 1 and 2 for the same orientation also showed increased growth for the WT except for the high toluene concentration in Study 2.

Overall, the results indicate that the coupling between transport of motile bacteria and population growth facilitated by uptake of toluene leads to a greater abundance of bacteria in the vicinity of the plume that will aid biodegradation in groundwater systems that are not naturally well-mixed.

Furthermore, it suggests the potential to engineer toluene-degrading bacteria toward greater toluene permeability for enhanced bioremediation efficiency.

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Augmentation of the chemotactic response of motile bacteria by coupling to flow paths within a porous matrix

Presenter: Roseanne Ford
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ABSTRACT

The transport of bacteria within a porous medium is critical for groundwater remediation, microbially-enhanced oil recovery, nitrogen fixation in legumes, and pathogenesis of disease. Of particular interest are motile bacteria that are able to swim toward increasing concentrations of chemicals that are beneficial to their survival. This ability to sense and respond to chemical cues in the surrounding environment is termed chemotaxis. In the context of groundwater remediation chemotactic bacteria migrate through the soil toward chemical pollutants, which they are able to biodegrade and utilize as carbon and energy sources.

At the pore scale individual bacteria sense and respond to chemical gradients that exist over distances of tens of microns while a bacterial population migrates over much greater distances in response to macroscopic-scale gradients. The chemotactic response of a bacterial population is characterized as an advective term at the Darcy scale, in which the driving force for the chemotactic velocity is a chemical gradient rather than a pressure gradient. Two transport parameters, the chemotactic sensitivity coefficient and the chemotaxis receptor constant, are used to quantify the chemotactic velocity.

Long and Ford (1) used a microfluidic device with an array of staggered cylinders as a representative porous matrix in which to study the chemotactic response of a bacterial suspension to a chemical gradient oriented transverse to the direction of the fluid velocity. They observed bacterial distributions for which the apparent chemotactic velocity was far greater than what was predicted by the transport coefficients that were determined in the absence of fluid flow. One possible explanation points to the coupling between the flow field and the swimming trajectories of the individual bacteria. As depicted in Figure 1, although bacteria may swim a relatively short distance across the width of a pore in response to a chemical gradient, by doing so they move from one set of streamlines to another, and are thereby carried a much greater distance in a favorable direction because the streamlines go around a cylinder with a diameter that is one hundred times greater than that of the pore space.

Upscaling by the process of volume-averaging leads to effective transport coefficients at the Darcy scale that incorporate characteristics of the velocity field and structure of the porous matrix. Porter and co-workers applied this process to the experimental data of Long and Ford (2), which yielded a better representation of the experimental data, but did not completely capture the magnitude of the chemotactic response. In this presentation we will explore further the unexpected results of Long and Ford (1) that yielded an apparent augmentation of the chemotactic response of individual bacteria to pore-scale gradients via coupling to flow paths within a two-dimensional porous matrix.

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Upscaling of bacterial transport in saturated porous media: The effect of flow from the pore scale to the Darcy scale.

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ABSTRACT

Understanding the transport of bacteria in saturated porous media is crucial for many applications ranging from the management of pumping wells subject to bio-clogging to the design of new bioremediation schemes for subsurface contamination. However, little is known about the spatial distribution of bacteria at the pore scale, particularly when small-scale heterogeneities – always present even in seemingly homogeneous aquifers – lead to preferential pathways for groundwater flow. In particular, the coupling of flow and motility has recently been shown to strongly affect bacterial transport1, and this leads us to predict that subsurface flow may strongly affect the dispersal of bacteria in saturated aquifers. We present here an upscaling framework for the transport of motile bacterial from the pore scale to the Darcy scale by combining detailed numerical simulations with controlled laboratory experiments. In particular, we show how the topological features of the flow correlate with bacterial concentration and promote the attachment of bacteria to specific regions of the pore network, which will ultimately influence the formations of biofilms. These results highlight the intimate link between small-scale biological processes and transport in porous media.

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Evaluation of bacterial cells transport in soil using laboratory column experiments

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ABSTRACT

Bacteria cells may present a risk for the environment and especially for aquifers. Most waterborne pathogens such as viruses or bacteria are of faecal origin, and come from human and/or animal wastes. Microorganisms are being increasingly released into the environment through human applications of solid wastes and contaminated wastewater effluents (e.g. manure, pit latrines, cattle grazing, sewage sludge spreading). The quality of aquifers can be affected by the movement of pathogenic bacteria, especially if water extraction wells are located close to soil surfaces subject to these land applications. These practices have led in some cases to calamities that demonstrate unexpected breakthrough of harmful microbes. On the other hand, industrial processes based on the injection of selected bacteria in the soil are emerging in the context of in situ bio-augmentation for soil bioremediation or bio-reinforcement. The efficiency of these soil treatment generally benefit from a uniform distribution of bacteria in the soil volume. However, defining optimal injection strategies remains very challenging. In both adverse and beneficial situations, it is thus crucial to improve our understanding of transport and retention of bacteria in porous media in order to predict and control their spreading in the environment.
In this context we studied the mobility of several bacterial species of specific interest (Agrobacterium tumefaciens, Escherichia coli, Cupriavidus metallidurans CH34, Pseudomonas putida and Sporosarcina pasteurii) in porous media using a column approach. The effect of various physical and chemical factors on the transport of the five bacterial species was investigated in saturated Fontainebleau sand columns. Some of these factors were shown to variably affect the mobility of these model bacteria (bacterial species, cell concentration, solution ionic strength and composition) while the others had much lower effects (cell size, pH and water flow) under our experimental conditions. The breakthrough curves of bacteria were well fitted with the advection – disperion model if accounting for irreversible cell retention. As a result, the longitudinal retention profiles of captured bacteria could vary drastically with the type of bacteria. Altogether these results showed that bacteria are variably mobile in porous media and that their mobility and ability to colonize natural porous environments strongly varies with the type of bacteria and is mostly controlled by the soil solution geochemistry

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Hiding behind an obstacle: bacterial accumulation due to flow-wall interactions.

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ABSTRACT

Flow surrounding an obstacle constitutes one of the classical problems in hydrodynamic [1], and it represents a simple model to understand complex systems as in the case of 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 Escherichia coli behind an obstacle (Fig. 1). 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 favor 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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Adsorption-Induced Deformation: Swelling and Shrinking

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ABSTRACT

When fluids are adsorbed on a solid surface they induce noticeable stresses, which cause the deformation of the solid. This phenomenon, called adsorption-induced deformation, is manifested e.g. in the swelling of coal during enhanced coal-bed methane recovery [1]. D. H. Bangham and co-authors concluded from a series of experimental measurements of adsorption-induced strains that physisorption causes expansion proportional to the lowering of the surface energy [2]. This statement is referred to as the Bangham effect or Bangham's law.

Here we show that even for physisorption Bangham's law is not always fulfilled, and that adsorption-induced deformation has to be described in terms of the change of the surface stress and not the surface energy. We use the BET (Brunauer-Emmett-Teller) theory [3] to derive both values and show the difference between them. We find the condition when the difference between the two vanishes, and Bangham's law is applicable. It is likely that this condition is satisfied in most of the cases, and prediction of strain based on the change of the surface energy is a good approximation. We show that this is indeed the case for adsorption of argon and water on Vycor glass. Finally, we show that the difference between the change of the surface energy and the change of the surface stress can explain some experimental data for adsorption-induced deformation of nanoporous materials that contradict Bangham's law and were therefore previously unexplained [4].

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A Multiscale Model for Enhanced Methane Recovery Incorporating Adsorption-Induced Coal Swelling

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ABSTRACT

Enhanced CoalBed Methane (ECBM) by CO2 injection consists of a tremendous unconventional gas resource environmentally sustainable which combines methane production with simultaneously CO2 sequestration. Coal seam is composed of a coal matrix containing pores of several nanometers with adsorbed CH4 and a natural fracture network (cleats) with high permeability often filled by water. Production of gas consists simply in reducing the pressure in the coal seam by means of a wellbore which first produces water from the cleats and subsequently gas desorbed from the matrix. The enhanced coalbed methane recovery consists of a CO2 injection process into the reservoir taking advantage of the huge adsorption and swelling potentials of the coal matrix. The modeling of the coupling between gas transport and poromechanics of the coal matrix is well reported in the literature and classically described by the Warren-Root dual porosity model combined with the Langmuir isotherm to compute gas adsorption in the coal matrix. In this work we consider the coupling between multiphase flow of binarygas components (CH4 and CO2) and water in cleats coupled with the swelling of a poroelastic matrix leading to the closure of the cleats induced by the simultaneous methane desorption and carbon dioxide adsorption. Macroscopic governing equations are derived by the homogenization method where we upscale the anomalous behavior of the binary gas mixture in the nanopores. The adsorption isotherm is constructed rigorously by exploring the Thermodynamics of inhomogeneous gases in nanopores. More precisely we consider nanopores of spherical geometries and apply the Density Functional Theory (DFT) to compute the gas density profiles incorporating both hard-sphere repulsion and Lennard-Jones attractive intermolecular interactions supplemented by a fluid-solid exterior potential. In addition we consider the mechanics of the matrix by computing the solvation force which induces the volume strain of the matrix. Finally a 2D reservoir simulation of methane production enhanced by CO2 injection is presented to illustrate the potential of the multiscale model proposed herein.

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Experimental characterization and modeling of coupling between swelling and permeability in coal

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ABSTRACT

Coal bed reservoirs naturally contain methane. During the production of this methane, the permeability of the reservoir is known to increase significantly, as a consequence of the shrinkage of the coal matrix and of the aperture of the coal cleats. Here we aim at characterizing experimentally and modeling those variations of the permeability of coal injected with carbon dioxide (CO2), used as a proxy for methane.

We perform a triaxial experiment on a cylindrical natural coal sample. Starting from dry conditions, pressurized CO2 is circulated through the core, while imposing isochoric conditions (i.e., the sample is prevented from deforming). We observe that, over time, compressive stresses increase, and the permeability decreases by about 2 orders of magnitude. Those observations are a consequence of the adsorption of CO2 in the coal micropores, which, if the sample was unconstrained, would make it swell.

We model how the presence of fluid can induce, for a constrained sample, 1) compressive stresses and 2) a consecutive decrease of permeability. The first part of the model is in fact a poromechanical model extended to adsorption effects, which is calibrated on swelling experiments during which a coal sample free of stress is pressurized with CO2. The second part of the model is calibrated by performing permeability measurements of coal under various states of stresses. As a whole, the model captures well the experimental observations.

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Mixed Hybrid FEM of Lanir Model in Finite Deformation

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ABSTRACT

Osmoelastic media have large negatively charged groups attached to the solid matrix. Due to the fixed charges, the total ion concentration inside the medium is higher than in the surrounding fluid. This excess of ion articles leads to an osmotic pressure difference, which causes swelling of the medium. Lanir's osmoelastic model assumes that small ions are always in equilibrium with the external salt concentration. This means that ion contribution is neglected and the medium is described by two constituents only: the solid and the fluid. In this paper, we implemented Lanir model using MHFEM (Mixed Hybrid Finite Element Method) for consolidation and free swelling experiment in both 1D and 2D cases, with result verification with analytical solution in 1D. The main advantage of MHFEM is that the local mass conservation is naturally guaranteed, see reference. The constituents are assumed to be incompressible. The infinitesimal deformation case has been investigated and the simulation results are compared with the analytical solution. In this paper, we focus on extending our solution method from infinitesimal to finite deformations. The material is assumed to be hyperelastic, isothermal, isotropic, homogeneous and fully saturated. Figure 1 and 2 are the simulation results of a swelling quarter of square sample in two dimensions. Figure 1 shows the geometry of the sample changing over the time, whereas figure 2 indicate the change in chemical potential in the up-right corner over the time. The material property of the sample is tuned to imitate the behavior of soft hydrogel and the swelling is induced by the decrease of ion concentration in the solution which comes in contact with the sample only at the right and top edges.

The system of equations consists of balance of momentum, fluid contents and Darcy's law, as shown in figure 3. Note that bold "T" denotes the macroscopic Piola stress, subscript 0 denotes the gradient taken with respect to the original configuration. "J" denotes the volume change of the mixture and varphi denotes the fluid volume fraction in the current configuration and bold "Q" is the fluid mass flow per unit volume of the initial mixture. Hence, equation (2) says that the change of the volume of the fluid in the mixture per unit of the original mixture volume is due to the in/out fluid mass flux per unit of original mixture. Bold "K" denotes the hydraulic permeability in original configuration and "k" is the Eulerian hydraulic permeability."mu" is the chemical potential, where "p" is hydraulic pressure and "pi" is osmotic pressure (deformation dependent). After we choose proper boundary conditions, derive weak formulation, linearize the system and compute the tangent stiffness with chosen interpolation functions and hybridization we end up with solving a (linear and discretized) saddle point problem. Backward Euler time integration scheme is employed and the program is implemented in MATLAB.

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Crack propagation in swelling media

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ABSTRACT

Ionized porous media, such as gels, clays and soft tissues, consist of a deformable porous solid matrix which is fully or partially saturated with fluid inside. They swell or shrink under changing osmotic conditions, and which can easily lead to cracks or discontinuities within materials. In return, the presence of discontinuities can also influence the mechanical behaviors of the porous media, like swelling capacity. Therefore, the study of fracture mechanics in swelling media is inevitably needed in several fields.

In the last decades, several mechano-electrochemical model including effect of ion concentration and ion flux were developed to represent swelling behavior. Lanir[4] developed a biphasic model of swelling assuming Donnan equilibrium with external salt solution, Lai et al. [2] derived a triphasic model that includes three phases (an incompressible fluid, an incompressible solid and a monovalent ionic phase) in small deformation. Later on, a finite deformation theory was presented by Huyghe and Janssen [3]. In the present paper, we present a partition-of-unity formulation of crack propagation with Lanir's model of osmoelasticity in finite deformation.

The total stress is divided into the effective stress part and the pressure part. The pressure part is the sum of the chemical potential and the osmotic pressure, which induce the swelling phenomenon. In order to introduce swelling, Van's Hoff empirical relation is used to describe osmotic pressure that is the difference between the internal and external osmotic pressure.

Considering cracks inside swelling media, a general partition of unity based cohesive zone model is exploited in conjunction with a discontinuous mode to avoid mesh re-generation during crack propagation [1]. Here, the crack is represented by a jump in the displacement filed of the continuum elements. The magnitude of the displacement field is governed an additional degree of freedom. Similarly, the chemical potential discreption within crack is treated the same way as displacement field.

In this paper, a finite deformation numerical model has been derived to study the crack propagation during swelling. The partition of unity method is used to introduce discontinuities into swelling media to study the interplay between fracture and swelling at the same time. A simple simulation is used to illustrate the mechanism of swelling and crack propagation. Figure 1 is the geometry and boundary conditions of a porous plate. A 0.4mm crack is present in the middle of the plate (l: 5.2mm, h: 10mm) with mesh size of 0.08mm×0.076mm. Figure 2 is the simulation result of chemical potential distribution and crack opening. The crack propagated without application of an external mechanical load.

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Laplace Transform Finite Element Method for Unsaturated Flow Problems in Swelling Media

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ABSTRACT

Incontinence products consist primarily of layered porous media, with each layer designed to be relatively thin and deformable for the sake of comfort. Furthermore, at least one layer, commonly referred to as a storage layer, undergoes swelling to about three times its original thickness as urine is introduced to the product and absorbed into hydrogel – in-plane swelling is relatively minor and typically ignored. Mathematical modeling of the combined problems of deformation, swelling and unsaturated flow throughout the entire product can only be solved through numerical methods – most commonly a finite element method to discretize the layered structure, together with a standard implicit ODE solver package to march forward in time, but designed to cope with the likely numerical stiffness of the ODE set. In spite of the availability of good ODE solver packages, there still is a need for robust and efficient time integration schemes, given that tens of thousands of elements may be involved. Here, we illustrate the use of Laplace transform methods to integrate the stated problem forward in time. After first building appropriate finite element equations on a suitable pentahedral mesh, sufficiently small time step sizes are utilized so that resulting finite element equations are linear and contain only "time-independent" coefficients. To simplify further, unsaturated flow and deformation events are treated as uncoupled – the entire medium is kept confined during swelling and unsaturated flow events, each lasting for about 10 μsec; subsequently, stress developed during confined swelling is relieved to yield incremental layer growth. After first applying the Laplace transform to the set of finite element equations, a standard band solver for linear systems is used to obtain dependent variables at each finite element node in Laplace space. Subsequently, the Stehfest(1) algorithm for Laplace inversion is used, with inversion based upon a 14-term sum(2). Since each term in the sum can be computed independently of the others, the overall inversion can be parallelized – using 7 or 14 cores, leading to considerable speedup since solving for nodal dependent variables in Laplace space together with inversion heavily dominates CPU usage. A number of numerical examples will be discussed in the context of evaluating absorbent behavior of incontinence products, which nominally consist of two or more physical layers – a non-swelling upper layer meant primarily for temporary liquid storage; and, a lower layer that contains components able to swell and permanently store liquid.

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Pore-scale modelling of swelling porous media

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ABSTRACT

Swelling of partially saturated porous media is a common and important phenomenon in industrial products, for example in paper, and hygienic products. To model flow of water in a dry granular porous media that can swell, one needs to go beyond current models which simulate either two-phase flow in porous media or mechanical behaviour in granular media. Current pore-scale models for two-phase flow such as pore-network models are tailored for rigid pore-skeletons, even though in many applications, namely hydromechanical coupling in soils, printing, and hygienic products, the porous structure does change during two-phase flow. On the other hand, models such as Discrete Element Method (DEM) which simulate the deformable porous media, have mostly been employed for dry or saturated granular media1.

In order to model the swelling of granular porous media at the pore scale, a two-phase flow model was developed and coupled with DEM. The aim is to simulate dynamic imbibition in a dry bed of so-called SuperAbsorbent Polymers, which are hydrophilic polymers capable of swelling 10's to 200 times their initial weight2. Subsequently, the swelling of a bed of particles is simulated using Yade-DEM. Such a pore-scale model allows for testing of continuum-scale approaches and it also provides an in-depth understanding of pore-scale processes responsible for effects at the continuum-scale.

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Preliminary investigation of fracture transmissivity in unconventional shales as a function of CO2 induced swelling

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ABSTRACT

Production of unconventional shale resources has increased dramatically as hydrocarbon extraction techniques have improved. These same techniques have also allowed for the consideration of carbon capture and utilization strategies in these reservoirs to promote both recovery and provide a long term storage solution for anthropogenic carbon.

Unconventional black shale reservoirs are prolific producers of hydrocarbons, including methane (CH4). These formations may also facilitate carbon dioxide (CO2) storage as the mechanisms by which CO2 partitions in these shales are analogous to CH4; CO2 also has a higher affinity for these rock types and will preferentially desorb CH4. Studies evaluating the mechanisms and quantities of absorption of CH4 and CO2 in these formation types have concluded that the absorption of CO2 is comparable (of the same magnitude) to that of methane and a function of swelling clay and organic content1,2.

Although some of the fundamental processes for CO2 uptake have been studied by pure mineral phases (e.g. illite and kaolinite) and select crushed shale samples, the resultant effects on shale structure and matrix swelling induced by CO2 uptake and subsequent fracture flow properties have not been evaluated in great detail. Coals swell and experience significant mechanical changes as a result of CO2 adsorption; this phenomenon may occur in organic rich black shales. It is crucial to understand these processes as it could lead to possible reservoir damage and impact the amount of petroleum recovered and total CO2 storage.

In this study, the transmissivity evolution of fractured Bakken and Marcellus shales exposed to CO2 were evaluated in a traditional core flow setup. Computed Tomography (CT) was used to observe bulk mechanical changes, and differential pressure was measured using single phase liquid CO2 flows to calculate transmissivity. The samples were characterized for bulk composition using X-ray diffraction (XRD), electron microscopy, and total organic carbon (TOC) analysis. Dual beam focused ion beam scanning electron microscopy (FIB-SEM) was utilized to discern microstructural features below the resolution of the CT scans.

CT scanning revealed negligible changes in the fracture aperture and shale structure. However, flow studies confirmed a reduction in permeability, suggesting a bulk decrease in fracture aperture that could be attributed to swelling. The causes of the matrix swelling are under investigation; however, CO2 sorption on the organic matter in the shale is the most likely cause of matrix swelling for the Bakken shale. The XRD data did not show the presence of swelling clays with the clay fraction being

dominated by illite and mica. The TOC ranged from 2.3% in the Marcellus shale samples to nearly 20% in Bakken shale samples. FIB-SEM analyses showed the presence of kerogen-rich regions with varying morphologies that are nonporous, pendular, and spongy in nature; organic porosity by volume was approximately 2% and 11% in Marcellus and Bakken shales respectively.

These analyses illustrate the physical properties and responses of fractured unconventional black shales to CO2 exposure. Future work will focus on identifying specific components that are contributing to swelling.

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Analysis, Efficiency, and Accuracy of Multirate Iterative vs Explicit Coupling Schemes for Coupling Flow with Geomechanics

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ABSTRACT

The coupling between subsurface flow and reservoir geomechanics plays a critical role in obtaining accurate results for both environmental and petroleum engineering applications [1]. The geomechanical effects, as a result of the influence of deformations in the porous media driven by the changes in pore pressure, can be very important especially in the case of stress-sensitive and fractured reservoirs. The fact that fractures present in porous media can severely influence flow profiles and subsequently mechanical deformations motivates the development of efficient and convergent coupling schemes for coupling flow with geomechanics in fractured reservoirs. Due to its physical nature, the geomechanics problem can cope with a much coarser time step compared to the flow problem. Multirate coupling schemes bridge this gap by exploiting the different time scales of the mechanics and flow problems and allow for taking multiple finer time steps for flow within one coarse mechanics time step. In this work, we first formulate multirate iterative and explicit coupling schemes for coupling flow with geomechanics in poroelastic and fractured poroelastic media. A quasi-static Biot model is assumed, in which fractures are treated as possibly non-planar interfaces, or lower dimensional geometrical objects. For iterative coupling schemes, our analysis is based on studying the equations satisfied by the difference of iterates, and is an extension of the work in [2] and [3]. By a Banach contraction argument, we prove that the corresponding iterative scheme is a fixed-point contraction. In addition, the analysis provides the values of adjustable coefficients used in the proposed schemes. For explicit coupling schemes, we consider stability rather than convergence, and show that for both single rate and multirate explicit coupling schemes, our computed solution remain well-behaved as long as the initial date are well-behaved. We then compare the efficiency and accuracy of both coupling approaches. Numerically, we observe that multirate explicit coupling schemes reduce run time efficiency, with an acceptable level of accuracy compared to their counterpart iterative coupling schemes. However, the accuracy and time savings of explicit coupling schemes over iterative coupling schemes are problem dependent.

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A model for sorption-induced swelling of porous media

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ABSTRACT

Swelling of porous media and materials due to sorption is a well-known phenomenon, which occurs in clay, polymers, gels, printing papers, biological tissues and many other materials and media. We study swelling of a disordered porous medium due to the sorption of fluids and fluid mixtures in the matrix. A thermodynamic theory based on the total energy of the system, which takes into account solid-fluid, fluid-fluid and solid-solid interactions, is used in order to couple the fluids and the solid matrix. The porous medium is represented by disordered matrix within which the pores are distributed. The fluids exert internal forces on the porous matrix and cause their deformation and swelling. Likewise, the deformation of the matrix affects the fluids' behavior in the pore space. Minimizing the total energy of the system with respect to the density of fluids and the strain, we obtain the equations of equilibrium, which we solve by the finite-element method.
We have computed the sorption isotherms as a function of the fluids' chemical potential, the moisture content, the strain, and the porosity of the matrix. Both single- and two-component systems have been studied.

Development of an accelerated test method for assessing gypsum efflorescence risk on clay brick masonry

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ABSTRACT

Gypsum efflorescence (GE) on ceramic brick masonry is on the rise, with more buildings being affected every year by this surface blemish. Regardless of GE's aesthetic impact only, this problem constitutes a considerable threat for the ceramic brick industry. Even though GE has been recognized for more than 3 decades (Chwast et al. 2015), a method for its assessment nor a solution to the problem is available. Salt crystallisation tests are widely applied to porous materials, however when adapted to GE reproduction they fail (Franke and Grabau 1998), or take too much time (Bowler and Winter 1997).

The main aim of this study is hence to develop an effective test method which allows investigating factors responsible for the recent GE occurrences. Such method should reproduce GE within a reasonable period of time as well as be versatile. It should thus be easily adapted for testing (i) brick and cement as GE sources, (ii) effect of brick transport properties and (iii) mortar admixtures as potential factors triggering its abundant formation (Chwast et al. 2015).

The method is developed based on a wick test, where a porous material (transport medium) is placed in a dish with a test solution (salts source). During the test (35°C, 20% RH) evaporation takes place solely over the brick core's (transport medium) top surface, resulting in a continuous flow of salt solution and salts crystallisation. Our first trials have confirmed that a basic wick test does not result in gypsum deposition over the surface, but rather within or under, forming subflorescence instead. The method was hence modified to simulate rain episodes, by interrupting the wick process with frequent wetting steps. Effectively, this wick-wetting yields a considerable GE formation. The brick core is connected to the setups lid with a sealant. It is of great importance to cautiously choose the sealant type, as the commonly used silicones may greatly interfere with the gypsum crystallisation process, inducing formation of abundant crusts. It was hence decided to seal the setups with a hot-melt solvent-free sealant. Additionally, the brick core samples are subjected to a leaching procedure prior to the test. This treatment reduces the undesirable interference of salts originating from the brick cores. The brick cores' surfaces are frequently photographed and the pictures are afterwards subjected to an image analysis procedure, allowing quantifying the efflorescence extent and its development tendency.

The applied tests have revealed a complex nature of the GE problem. Both bricks and masonry mortar may contain GE sources. While these may be directly available in bricks, in mortar the GE source is formed upon carbonation. Nevertheless, GE source presence itself is not sufficient to yield abundant deposits as observed under field conditions, as gypsum exhibits an intrinsic pore clogging tendency, limiting the possible GE extent. This tendency can be overcome in presence of surface active mortar admixtures, which in turn can be deactivated when bound in a cement matrix.

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Drying kinetics and subflorescence in Plaster

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ABSTRACT

Building materials are often subject to drying-imbibition cycles which induce transport and concentration of species (ions, colloids) modifying material properties and altering performance. Moreover, in the making process, for workability purposes, a surplus of water is added, which must be evacuated by evaporation after setting. In the case of plaster 80% of the initial water remains at the end of the setting.
We show that plaster dries significantly slower than an equivalent model porous media filled with pure water. In the case of imbibition-drying cycles, the drying rate is reduced by orders of magnitude. Indeed the liquid in the plaster porous structure is not pure water but a saturated ionic solution. As water is transported toward the free surface, the local concentration increases and leads to crystallization. Crystals reduces the local porosity at the free surface.
Further investigations by MRI and X-Ray microtomography provide information on the crystal formation and liquid distribution which help us understand the mechanism of crystallization during drying. Crystals develop at the first air/liquid interface under the free surface. These crystals act as a dewetting agent and the liquid front recedes. Thus water vapor diffuses over an increasing length thus reducing the drying rate. We could directly visualize these mechanisms by optical microscopy on glass channels saturated with calcium sulfate solutions. Finally we propose a simple physical model which is able to predict the drying kinetics and crystal localization.

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A 3D microscale model for predicting the heat flow through porous building materials

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ABSTRACT

Highly porous materials find frequent use in numerous thermal applications, due to their relatively high resistance to heat transfer. Typical examples include the automotive industry and aerospace engineering for the protection of thermally sensitive components, but also the building industry to reduce the heating energy demand of buildings. However, with the built environment still being responsible for almost 40 % of global CO2 emissions, better performing thermal porous building materials are highly necessary.

The heat flow through such materials is usually described with Fourier's law using the macroscopic effective thermal conductivity (ETC), while in fact it originates from the aggregation of several complex heat transfer mechanisms at the pore scale: conductive heat transfer through the matrix and through the gaseous phase in the pores, thermal radiation between the pore walls and convective heat transfer via the gaseous phase. The relative contribution of these heat transfer mechanisms depends strongly on the microstructural parameters, i.e. porosity, pore size, matrix connectivity etc. [1,2]. A correct understanding of the direct relation between these microstructural parameters and the total heat transfer is therefore crucial in the development of improved thermal materials. However, current models attempting to study this influence still exhibit large errors due to 2D simplifications, neglect of thermal radiation or their very limited applicability for a restricted class of materials.

This study presents a newly developed 3D FEM model for simulating the heat transfer through a porous structure on the micro-scale. The model is based on 3D voxel images of the material as input for the meshing code, hence ensuring the incorporation of the true microstructural parameters. Moreover, this approach allows performing simulations on both real materials using micro-CT scanning and synthetic materials using random generation algorithms. Other needed geometrical parameters are acquired from the 3D voxel image via a set of image processing routines. After the meshing procedure the heat flow is simulated using a finite element code. A method for modelling thermal radiation as a diffusion process at the pore scale is investigated, resulting in a definition of a radiative conductivity coefficient as a function of geometrical and physical parameters.

The model is validated by comparing the simulation results of several elementary pore structures with the values given by conventional analytical models and other numerical simulation packages, showing good agreement. An in-depth study of the influence of the mesh and voxel discretization is performed for a correct and optimal use of the model. Subsequently, the model is used for a preliminary study on the influence of different material parameters, including porosity, pore size distribution, ratio of solid and gaseous thermal conductivity etc. This results in a clearer understanding of the microscopic parameters and their effect on the macroscopic thermal conductivity.

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Absorption of water droplets impacting natural porous stones

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ABSTRACT

The phenomena of drop impact, spreading, absorption and redistribution on three natural porous stones frequently used in building façades, Savonnières, Meule and Pietra serena, are experimentally determined using high-speed imaging and neutron radiography.

During impact and spreading, the droplet exhibits a dynamic non-wetting behavior. The dynamic non-wetting behavior during spreading and the hydrophobic dynamic contact angle > 90 degrees is attributed to the presence of an air layer between droplet and porous substrate. As the contact line pins at maximum spreading on porous stones, the maximum spreading determines the liquid contact area on such substrate. The droplet gets pinned when the air layer is broken at the contact line and capillary forces develop in fines pores at the droplet edge pinning the droplet.

Maximum spreading on porous stones increases with impact velocity but does not scale with Weber number at low impact velocity. It is demonstrated that dynamic wetting plays an important role in the spreading at low velocity and that the dynamic wetting as characterized by the dynamic contact angle has to be taken into account for predicting the maximum spreading. Correcting the maximum spreading ratio for the dynamic wetting behavior, it is demonstrated that all data for porous stones and non-porous substrates collapse onto a single curve.

The absorption process of an impinging droplet is fully characterized from spreading to evaporation in terms of absorbed mass during droplet depletion and moisture content distribution in a time-resolved manner for three different natural stones. High-speed imaging and neutron radiography are used to quantify moisture absorption in porous stones of varying moisture properties from deposition until depletion. At maximum spreading, as the droplet undergoes pinning, the contact radius remains constant until droplet depletion. Absorption undergoes two phases: initially, absorption is hindered due a contact resistance attributed to entrapped air; afterwards, a more perfect capillary contact occurs and absorption goes on until depletion, concurrently with evaporation and further redistribution.

Droplet spreading and absorption are highly determined by the impact velocity of the droplet, while moisture content redistribution after depletion is much less dependent on impact conditions.

Figure. Schematic representation of the fate of a water droplet impacting on a porous medium

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Spatially-resolved investigation of heat of sorption in hygroscopic porous materials

Presenter: Dominique Derome
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ABSTRACT

Water adsorption (desorption) in a hygroscopic porous material is accompanied by a release (intake) of energy. Due to the small quantities involved, this process has yet to be properly characterized. In this study, we combine neutron imaging experiments and numerical modeling to gain insight regarding the heat effects associated with sorption.
Moisture content variations in three porous materials, i.e. cellular concrete, plaster and wood, are imaged at high resolution with cold neutrons at the ICON beamline of the Paul Scherrer Institute (Villigen, Switzerland), while simultaneously monitoring the temperature variations within the materials with thermocouples, to identify sorption as a source/sink of heat.
Samples measuring 88 x 35 x10 mm3 are pre-conditioned to be dry in oven or moist at equilibrium at 90% RH. The samples, thus of known initial uniform moisture content and uniform temperature of 23 degC, are mounted inside a micro-wind tunnel with their sides sealed, leaving only the top surface exposed to the controlled air flow. The tunnel is mounted on a high precision balance to acquire mass in real time. The wind tunnel is designed to have a minimum mass and allowing placement of the samples close to the detector. In this very controlled experiment, moisture content distribution is imaged at high resolution with cold neutron radiography, while simultaneously monitoring the total mass and the temperature variations within the samples. The samples are then subjected to a step change by exposing them for two hours to a 0.3 m/s or 1.0 m/s flow of moist air (90% RH and 23 degC) for dry samples or of dry air for moist samples, resulting in a sorption or a desorption process respectively. Neutron radiography, temperature and mass data are acquired every 20 seconds for the whole duration of the adsorption/desorption process. The data was acquired over two beamtimes.
The two-dimensional temperature effect during sorption/desorption is shown and moisture content variations in wood, cellular concrete and plaster are successfully imaged. The mass data provide the total moisture content variation simultaneous to the 2D moisture content field for the duration of the experiment, allowing further calibration. Twin experiments in the laboratory, so without imaging, are conducted on the same samples to ensure reproducibility. Experiments illustrate a higher moisture load and a more pronounced temperature effect on the downstream part of the sample. Also, a clear temperature variation, totally due to water sorption, is observed over the sample depth, related to moisture content variation.
In addition a two dimensional numerical model considering heat and moisture transport in the air

domain together with the porous material domain is developed and validated against measurements. The validated finite-element based model is used for parametric studies, to better understand the impact of environmental conditions (air velocity, relative humidity, temperature) on thermal effects associated with sorption.

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Multiscale CT evaluation of laboratory and field samples as a proxy for wellbore foamed cements

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ABSTRACT

Foamed cement, a light-weight alternative to traditional wellbore cement, is widely used for casing oil and gas wells in high-stress and deep offshore environments. Despite common usage, significant knowledge gaps exist in terms of cement properties at in-situ wellbore conditions. Analysis of foamed cement in its downhole environment presents a unique set of challenges. The placement process, with foamed cement slurry created at the surface and then pumped downhole, as well the deep subsurface conditions at which the cement cures, play a role in determining porosity, permeability, and mechanical strength of the final cured cement. While obtaining samples from actual wellbore cements is difficult and costly, wellbore safety makes it imperative that such cements be well-understood. In this overview, several methodologies for obtaining foamed cement samples were evaluated, and computed tomography (CT) scanning at a range of scales was utilized to compare and contrast samples in terms of their representativeness and usefulness for informing industry safety standards.

Samples were generated in three distinct ways, with a range of entrained air qualities. Atmospherically-generated cement samples were mixed and cured at room temperature and pressure conditions, per American Petroleum Institute's recommended practice 10B-4. Samples of cement at pressure were generated with a small-scale laboratory system (De Rozieres and Ferriere, 1991). Finally, field-generated foamed cement samples were collected in 3-ft vessels in cooperation with industry partners using actual industrial field equipment at field conditions. Small laboratory cement samples were imaged using an industrial CT scanner at resolutions ranging from 3 to 25 µm. Large field samples were first imaged whole in a medical CT scanner at a coarse resolution of ~450 µm. They were then subsampled to permit higher resolution scanning. Samples were characterized in terms of the distribution of entrained air, and the resulting porosity, permeability, and mechanical characteristics.

Atmospherically generated foamed cements exhibit largely homogenous entrained air distributions, porosities, and permeabilities, but are the least representative of downhole conditions. Laboratory-generated pressurized foamed cements display heterogeneity in terms of both the permeability and entrained air void distributions generated during the collection procedure. Field-generated cements range widely, from homogenous to very heterogeneous in terms of entrained air distribution, porosity, and permeability. Field-generated cements are likely to be the most representative of wellbore conditions, but are as with laboratory samples, they are likely affected by collection procedures. While high-resolution imaging is crucial to understanding the entrained air distribution at a small scale, it is most effective for evaluation of homogenous laboratory samples.

Field samples exhibit heterogeneity at a coarse scale, requiring a low-resolution imaging approach for proper characterization.

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Understanding the residence time of water in porous asphalt

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ABSTRACT

Porous asphalt (PA) is a special type of asphalt concrete with a high porosity of about 20% by volume. Porous asphalt is used effectively to improve driving conditions under rainy weather (reduction of aquaplaning risk) and the quality of the aural environment, given the noise reduction properties of this material. However, due to its high porosity, more surface area undergoes the detrimental effects of the environment leading to a life expectancy of around 10 years, compared to 20-30 years for dense asphalt concrete. A key issue in understanding PA, and in improving its durability and mechanical performance, is a thorough portrayal of its wetting and drying behavior under environmental loads, specially of the time of residence of water within the porous asphalt. We developed an integrated multiscale methodology, based on a combination of experimentally validated models, to capture accurately the main physics of the wetting and drying of porous asphalt at the material scale (pore scale), and that can be used in road engineering at the pavement scale (macro scale), in the development and assessment of pavement solutions, as shown in the attached Figure.

The geometry of porous asphalt presents a network of highly connected larges pores, in the millimeter range. The surfaces of the pores are highly irregular and rough, due to the nature of the aggregates. The asphalt binder is bitumen-based and thus hydrophobic (approximately, with contact angle of 100°), until environmental conditions, such as ultraviolet radiation or presence of water, degrade its surface which can become hydrophilic (approximately, contact angle of 50°), with years [3]. We capture this geometry with X-ray microCT scans of different resolutions, analyze the structure in terms of pore size distribution, connectivity and observe that the range of pore size reaches to micrometers.

We study the water behavior of individual pore or systems of pores using Lattice Boltzmann modeling (LBM) [1] to capture the liquid/gas interface and to particularly observe challenging unsaturated phenomena such as liquid flow through grooves, corner flow and dead-end pores. We also perform the gravity-driven drainage in large pore systems studied by the LBM and compare with microfluidic experimental results.

We perform different wetting of porous asphalt by pouring water or sprinkling droplets, drainage from saturated state and drying with controlled air conditions using a small wind tunnel and radiative heat source. We document the variation of liquid content using neutron radiography [2] and attain high moisture-content and spatial resolutions of the configuration of liquid water in this complex geometry. We also study vapor transport in porous asphalt with CFD simulations using a real PA geometry from X-ray μ-CT scans. We model the wetting and drying of porous asphalt with pore network and upscale to continuum scale.

We thus look into the physical phenomena related to moisture and its residence time underlying the process of deterioration. With the emergence of modern experimental and analytical techniques, it is possible to look into the problem using advanced experimental and modeling techniques that leads to a deeper understanding, essential for practical solutions.

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Pore-scale study of fluid flow and mass transport in carbon fiber electrodes of vanadium redox flow batteries

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ABSTRACT

The U.S. has increasing needs for energy storage in its electrical power grid because of the increasing use of renewables that produce power intermittently. Among multiple forms of energy storage, flow batteries hold the greatest promise for next generation grid-scale energy storage technology. Although various technologies are being developed to increase the power density and energy storage density of flow batteries, a fundamental modeling effort has thus far been lacking in flow battery research with the goal to optimize material design and architectures. Such optimizations can have an impact on the power density by nearly an order of magnitude.

We present a pore-scale numerical study of coupled electrolyte flow, ion transport, and electrochemical reactions in the carbon fiber electrodes of vanadium redox flow batteries. Ion transport and electrochemical reactions are simulated and the reaction efficiency is predicted. With simulations on about 200 samples, effects of carbon fiber diameter and porosity on the permeability and effective diffusivity of the electrodes are investigated in detail. Reaction efficiency under different flow and reaction rate constants is also predicted. Structures of the carbon fiber electrodes are optimized to reduce the flow resistance and at the same time obtain acceptable reaction efficiency.

Direct Visualization of Electrochemical Reactions in Porous Carbon Electrodes by Fluorescence Microscopy for Organic Redox Flow Batteries

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ABSTRACT

As our world transitions to renewable energy generation technologies, massive energy storage systems are being investigated to make these inherently intermittent energy sources dispatchable at will. Aqueous organic redox flow batteries present a potentially cost-compelling solution for these challenges, yet this nascent technology has numerous opportunities for substantial improvement. Aqueous flow batteries are non-flammable and allow the decoupling of stored energy and generated power for long-duration sustained-power operation; using redox-active organic electrolytes enables non-toxic, inexpensive chemistries with tunable properties. The battery hardware, however, remains a carryover from fuel cell technology—particularly porous carbon electrodes and ion-selective membrane separators. Understanding how these materials function in organic redox flow batteries, and how they can be improved, will be important for advancing this technology.
Using fluorescence microscopy we directly visualize the redox reactions of soluble quinones within porous carbon electrodes. We show this technique can be used to map the state of charge within flow battery electrodes with areas >2cm2 and to see within the electrode pores at <100 ?m resolution. Furthermore, we are able to explore dynamics at time scales ranging from 10s of milliseconds to minutes or longer, allowing for both high-resolution, high-speed analysis and large-area, time-lapse studies. This technique can be used to rapidly evaluate the spatial-temporal effect of porosity and electrode structures on organic redox battery performance informing futures designs of flow battery hardware.

Design of nanoporous materials with optimal electrochemical properties

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ABSTRACT

Macroscopic models of electrochemical transport are essential for design of porous electrodes for super-capacitors and batteries. We introduce such a model to simulate transport in, and optimize performance of, hierarchical porous materials with meso- and micro-pore structures. An advantage of hierarchical porous materials is their ability to form an extensive electrical double layer (EDL) over large accessible surfaces by facilitating diffusion of electrolyte ions into the interior surface. Our model is derived by homogenizing the microscopic behavior of binary monovalent electrolyte solution in nanoporous material. This behavior is described by a mass conservation equation coupled with an electric potential distribution Poisson-Boltzmann (PB) equation. The model relies on a microscopic closure relation between the microscopic electric potential distribution and the pore-scale structure, which satisfies a local PB problem in a periodic unit cell. By expressing the effective properties of nanoporous materials in terms of their microscopic counterparts, our model enables one optimize the former by using the latter as decision variables and, hence, design the next generation of materials for energy storage devices. It also provides a solid foundation for the empirical Bruggeman relation between a material's tortuosity and porosity. The effective diffusion coefficient and transference number in an EDL capacitor predicted with our model are in agreement with experimental data.

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Membraneless Batteries with Variable-Density, Immiscible Electrolytes

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ABSTRACT

Recent years have seen a large increase in renewable energy production. The Department of Energy has identified improved energy storage as necessary to expand renewable energy use. Due to the intermittent nature of renewable energy sources, these advanced batteries must have a large capacity and must survive many charge/discharge cycles.

Electrochemical cells contain four major components: cathode, anode, electrolyte, and membrane. Of these, the membrane is often the most expensive part of a battery and the most prone to failure. Consequently, improved membranes are an active research area. One solution to the membrane problem is to design batteries without membranes. Previously, bromine complexing agents and laminar flow have been proposed to as membrane replacements.

We introduce a membraneless hydrogen-bromide battery system which incorporates liquid bromine and phosphoric acid as electrolytes. The immiscibility and different densities of the fluids are leveraged to create a layered structure where the bromine/phosphoric acid interface serves to separate the cathode from the anode. The liquid electrolytes allow for the design of a flow battery, which offers easily expandable capacity, but unlike the laminar flow batteries, these batteries can be configured to operate without flow as well. The addition of porous structures inside the electrochemical cell can improve the stability of system, making these batteries suitable for mobile applications. In this work, we simulate the Nernst-Planck, Poisson, and Stokes equations to investigate the performance of the battery. Of particular interest are cell potential and the bromine/phosphoric acid layer thicknesses.

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Homogenization of Carbon-Nanotube Brush Electrodes

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ABSTRACT

Carbon nanotube brushes (carbon nanotubes attached to a current collector) have been proposed for nanoscale electrodes. While the detailed molecular scale physics is important in its own right, often a more useful scale to examine electrode performances is the micro and meso-scale continuum. The detailed structure of microscale material parameters results from statistical mechanics and will not be discussed in this talk, rather we focus on the micro-scale homogenization to the meso-scale wherein material parameters result from a micro-scale cell problem for a periodic lattice. We apply a matched asymptotic formulation to obtain the meso scale field equations and material parameters. The finite element method and finite volume method are employed to solve the micro scale cell problem and the mesoscale field equations, respectively. Numerical results will be presented for the electrical potential field and concentration of cations and anions.

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Hybrid, Membraneless, Variable-Density, Immiscible-Fluid Batteries

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ABSTRACT

We discuss a novel approach to battery design based on fluid properties such as density and immiscibility.
These hybrid batteries are membraneless and some can be used in either a flow or no-flow environment.
The basic idea is to choose a set of fluids that are of differing densities with fluid 1 immiscible with fluid 2 and fluid 2 immiscible with fluid 3 and etc. If necessary to each fluid add a salt or acid that disassociates within the fluid to increase its conductance (i.e. form an electrolyte). Layer the fluids so that buoyancy forces the lightest to the top layer and the heaviest to the bottom layer. Add current collectors/electrodes in a series or parallel arrangement. As examples we present three such systems:
System1 Hydrogen gas (at pt electrode)--phosphoric acid (fluid 1), liquid bromine with HBr acid (fluid 2);
System 2 Hydrogen gas (at pt electrode)--ethyl acetate with tetraalkyammonium-Br salt (fluid 1), aqueous HBr (fluid 2);
System 3 Hydrogen gas (at pt electrode)--ethyl acetate with tetraalkyammonium-Br salt (fluid 1), aqueous HBr (fluid 2), propylene carbonate with bromine and LiBr salt (fluid 3).
To stabilize the batteries for mobile application, embed the electrolytes in porous structures while taking advantage of the solid phase characteristics.

Salt damage in wood

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ABSTRACT

When wood is frequently exposed to salt water or salt laden vapor, it is prone to salt damage. Salt damaged wood appears “fuzzy” and is and is sometimes mistaken for fungally degraded wood. The fuzzy appearance is the result of individual wood cells and bundles of cells being partially separated from the bulk of the wood.
Salt damage is not unique to wood and the mechanism for salt damage in porous stones mortars and concrete has been well studied. For these materials, the salt damage is a result of purely mechanical interaction. Salt crystalizes in small pores which creates a stress concentration that eventually causes cracks to form in the material. Poromechanics can be used to calculate when a salt crystal will form in a pore and whether or not it will cause cracking.
Previously, salt damage in wood has not been studied as much as in other porous materials. Several different possible mechanisms for salt damage have been proposed. The simplest mechanism is that salt crystallization causes mechanical separation of the cells [1]. However, Parameswaran proposed that the salt causes alkaline pulping of the wood fibers [2]. Salt damage preferentially damages the middle lamella, however, it is unclear whether this is for physical or chemical reasons since both the chemical composition and the physical structure (pore size) of the wood are different in the middle lamella.
Here we present preliminary research on salt damage in wood. The method of Scherer was used to recreate salt damage in the laboratory [3]. Specimens were partially immersed in a 5M NaCl solution within a humidity chamber held at 39%. Additionally, modifications to the test will be presented which are aimed at differentiating between different proposed mechanisms of salt damage in wood.

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Water sorption in wood cell S2 layer – Molecular Dynamics insights

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ABSTRACT

Adsorption of water and swelling are phenomena occurring in the wood cell wall, a porous and complex composite material. The thickest cell wall layer, S2, is composed of three types of polymers: cellulose, hemicelluloses and lignins. Cellulose fibrils, composed of crystalline and amorphous cellulose, give strength to the material, whereas lignin and hemicellulose play the role of soft amorphous matrix which glues the cellulose fibrils together. Amorphous cellulose, hemicellulose and, to a lesser extent, lignin are hydrophilic polymers: with increasing relative humidity, they adsorb water molecules causing a decrease of stiffness and overall swelling of the cell wall.

This study uses Molecular Dynamics (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 in order to mimic an infinite system. A typical time scale of a simulation is 10 ns with a resolution of 1 fs. The high spatial and temporal definition of MD method enables us to capture the complicated detailed behavior of wood cell materials.

Given the role of moisture in wood [1], we investigate in details, using Molecular Dynamics (MD) simulations, the system behavior when exposed to moisture, i.e. the mechanisms of swelling and material weakening. The construction of an MD model of S2 layer, followed by collection of relevant in-silico experiments and validation with experimental data, e.g. [2], gives insight into wood-moisture interaction at atomistic scale. We constructed and investigated a three-phase model of a cellulose microfibril aggregate that consists of crystalline cellulose, amorphous hemicellulose and lignin. Water molecules are adsorbed in the amorphous hemicellulose and lignin, with an excess of sorption at the interface, while no sorption occurs in the crystalline cellulose. As the moisture content increases, water molecules are adsorbed in the bulk amorphous phase, but also preferentially at the interface, leading to a swelling, proportional to the porosity increase and a mechanical weakening, related to the breaking of hydrogen bonds (Fig. 1a). Modeling results are shown in the Figure below.

The process of water adsorption and its influence on wood material are still not completely understood, specifically at the molecular scale. This work aims at elucidating the mechanisms of water interaction with wood cell wall layer at the nanoscale. Next steps for our S2 wood cell wall layer model are the inclusion of xylan and a more advanced model for lignin. Nevertheless, we have so far obtained by MD the molecular sorption curves for assemblies as well as for each polymer and for a S2 unit cell, performed evaluation of mechanical properties change within the hygroscopic range, and identified the mechanism of water sorption in assemblies in terms of cross-sectional water profile density and number of hydrogen bonds in polymer-polymer versus water-polymer bonds [3, 4, 5]. We have successfully upscaled the results using a poromechanical approach as per [6].

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Hybrid Mixture Theory based modeling of Fluid and Heat Transport During Frying of Foods

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ABSTRACT

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 comparison to the experimental data on moisture transport, heat penetration and pressure development during frying of potatoes and chicken nuggets. 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 mechanism were performed using image analysis of micro-CT images and by performing lab experiments. The results were used to make conclusions about modifying the frying process for obtaining healthier foods with reduced fat uptake.

Multiscale simulation of expanded starchy snacks

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ABSTRACT

We present a multiscale simulation on the expansion of food snacks, based on starch. Snacks like keropok or Pringles are made via frying of relatively dry pellets made of starch. Because of the intense heating during frying, the moisture is converted into steam which expand upon further heating. If the bubbles show partial rupture, steam can escape and the starch matrix will be fixated as it undergoes a glass transition. Via this process a porous, crispy, solid foam product is obtained. We have developed a multiscale simulation model in order to understand this complex process, and to obtain product design rules for reduction of salt levels [1,2].
The multiscale model describes the system on three levels: micro-, meso, and macro-level. On the (molecular) microlevel we describe the thermodynamics and diffusion kinetics of the system – using predictive theories based on free volume theory and Flory-Huggins. At the mesoscale we describe the expansion of a single bubble using a cell model based on a momentum balance. The driving force for expansion is the steam pressure, which directly follows from the thermodynamics of the dry starch matrix. Expansion is hindered by the matrix viscosity, which is directly related to the matrix glass transition. From the mesoscale model follows the porosity, which is fed to the macroscale model – describing the heat and mass transfer on the scale of a single pellet.
We have obtained sound understanding of the problem via interpretation of the simulation results in a state diagram, showing the boiling and glass transition. Expansion is shown to be optimal at the crossing of the two transition lines.
The model has been extended for snack formulations with different levels of salt. Addition of salt leads to change in both boiling and glass transition. Hence, to get optimal expansion moisture content needs to be modified accordingly.

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Structure of model protein gels and release of sodium

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ABSTRACT

Sodium reduction in protein/lipid-based products such as cheese is becoming increasingly important to the food industry. Since only a fraction of sodium is released from food matrices during oral processing, the effective release of sodium during oral processing may lead to a strategy to reduce sodium content in foods. Understanding the food structure critical to sodium release is one of the keys to effectively controlling the sensory quality of the product while lowering the sodium content.

Efforts have been made to relate sodium release to microstructural properties of solid lipoproteic colloid (SLC) foods. Model SLCs with 1.5% and 3.5 % (w/w) NaCl were prepared with whey protein isolate and anhydrous milk fat. The protein, fat, NaCl, and water were homogenized, and gels were formed by heat. The gels varied in protein content (8% or 16%), fat content (0%, 11%, 22%, or 33%), and homogenization pressures (14 or 55 MPa). Structural properties including porosity and protein and fat particle sizes were measured. The sodium release characteristics during single compression of the gels in water were collected. Serum release and texture of the gels were also analyzed.

The maximum rate of sodium release during the initial gel compression increased with increasing gel porosity. This relationship was due to more releasable serum in the gels with larger pore volume and larger pores. The maximum concentration of sodium toward the end of sodium release profile was affected by the size of the fat particles more than the porosity of the gels. The smaller fat particles were dispersed more uniformly and interrupted the protein network more, and facilitated the gel breakdown. The above findings suggested that, during the breakdown of the SLC gels, the major mechanisms of sodium release are via serum release followed by sodium diffusion, which are governed by the gel porosity and the particle size of fat, respectively. It was also suggested that the particle size of fat is a better indicator of sodium release than the size of emulsion particles. The relationship of sodium release properties and the microstructural properties of an SLC food system was demonstrated. The findings from this study could lay the foundation for further investigation of the dependence of saltiness perception on SLC microstructure, which can provide insight for sodium reduction in protein/lipid-based products.

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The Role of Internal Porosity on Large-Scale Transport through Porous Media

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ABSTRACT

Motivated by experimental observations by geophysicists, we develop an upscaled framework, based on the Spatial Markov model, for studying conservative transport and exploring the impact of internal porosity on larger scale transport phenomena through porous media. Stokes flow through idealized porous media at pore scale is modeled at high resolution using lattice Boltzmann methods; transport at this scale is modeled using standard random walk methods. In particular we consider two different transport settings: (1)- Periodic array of completely impermeable solid objects; (2)- The same array as in (1), but where the solid grains are themselves porous and allow transport through them. We then measure and predict breakthrough curves over large scales for a range of Péclet numbers, spanning diffusion to advection dominated behavior. We identify several interesting differences in breakthrough curves between the two model configurations that enable us to discern the impact of internal porosity on transport and better interpret the motivating geophysical data.

Statistical Description of Anomalous Transport from Geometric and Topologic Characteristics of the Pore Space

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ABSTRACT

Non-Fickian diffusion in heterogeneous porous media is a ubiquitous phenomenon that underlies anomalous transport and poses a challenge for making predictions. Various
physically-based models have been proposed to describe the occurrence of anomalous transport in porous media. Yet, the links between measurable structural properties of the pore space and observed anomalous transport behavior remain tenuous. This work experimentally identifies the statistical relationships between pore-space properties (in geometry and topology) with deviation magnitude from Fickian transport. Cubic flow-through cells packed with granular Nafion and an aqueous solution of matching refractive index (optically transparent) are used to create different realizations of heterogeneous porous media. First, flow is determined in the transparent flow-through cells by tracking the position of flowing tracer particles with a particle velocimetry technique. Statistical analysis of recorded particle trajectories is then used to determine flow dynamics within the pore space Second, the structural features of the pore space are characterized from X-ray Computed Tomography images analyzed in a network framework. Pore-space networks consist of nodes and edges of unique geometry, whose layout captures the topology of the pore channels. Spatially compatible information about the flow and the pore structure is then used to ascertain the following. a) Statistical properties of the pore space that are associated with heavy velocity distributions. b) The likelihood of presence of channels that act as shortcuts that cause superdiffusive displacement. And c) retrieve a function that relates particle residence times within a channel to the channel's geometric properties.

Non-Fickian Migration of Inert Particles on Stochastic Fracture Networks

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ABSTRACT

Geometrical attributes of fracture networks such as length distribution, orientation, and density influences the network connectivity and imparts dispersion to a migrating plume of particles. Though the rate of growth of plumes on fracture networks are usually thought to be non-Fickian, the extent of departure from Fickian behavior is intricately tied to properties of the fracture network. In applications where transport characteristics of fracture networks are desired on larger scales, important questions such as ergodicity of the system and early- and late-time growth dynamics are often of interest. A discrete fracture network model is constructed with steady state flow fields to track particles through two-dimensional stochastic fracture networks with realistic statistical attributes. Particles are modeled to move only by advection so that the plume dispersion is a function of network patterns and velocity distribution of individual segments. Rates of change in separation distance between particle pairs are utilized to characterize plume growth and scaling behavior for a set of networks with power-law fracture length distribution and density values ranging from sparse to dense. Given uniform transmissivity values for fractures in the system, smaller values of power-law exponent for length distribution favors a less dramatic shift from Fickian rates of growth. The analysis helps in understating suitability of Fickian versus Non-Fickian transport models for fractured systems at different length scales.

Computational models for Fractional Dynamical Systems

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ABSTRACT

In the last decades, fractional differentiation has played a very important role in various fields. In particular, in the field of Cardiac science, fractional models are used to explain the influence of tissue heterogeneity on cardiac wavefront propagation. Mathematical models of the heart can be used to simulate heart conditions and the effects of certain drugs designed to treat them. However, the extent to which electrical propagation is influenced by the highly complex, and heterogeneous nature of cardiac tissue remains unclear.

In this paper, two fractional FitzHugh--Nagumo monodomain models are presented, generalising the standard monodomain model that describes the propagation of the electrical potential in heterogeneous cardiac tissue.

Model 1: A fractional FitzHugh--Nagumo monodomain model [1] with space Riesz fractional operators on an approximate irregular domain [2].

Model 2: A fractional FitzHugh--Nagumo monodomain model with fractional Laplacian operator [3,4] on arbitrary irregular domains with unstructured mesh.

Firstly, we use decoupling techniques and focus on solving fractional dynamical systems on the Model 1 and Model 2. Secondly, an alternating direction finite difference implicit method is proposed for solving fractional dynamical systems on Model 1 with homogeneous Dirichlet boundary conditions on an approximate irregular domain. Thirdly,a control volume finite element method is introduced for solving fractional dynamical systems on Model 2 with homogeneous Neumann boundary conditions on arbitrary irregular domains with unstructured mesh. Finally, some numerical results are presented and these techniques are used for simulating Model 1 and Model 2.

We found that such models can have very different dynamics to the standard monodomain model and, as such, represent a powerful modelling approach for understanding the many aspects of electrophysiological dynamics in heterogeneous biological tissue.

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Fractional order Darcy law for fluid flow through porous media

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ABSTRACT

Fluid flow through porous media is a key issue in many areas of the science such as petroleum engineering. Several nonlinear models have been introduced to describe Non-Darcy fluid flow through porous media, and have achieved great success in many cases. However, parameter determination and physical mechanism are still open issues in modeling of Non-Darcy fluid flow through porous media. Here we employ fractional derivative to characterize the history memory and nonlocality feature of particle movement in heterogeneous media, and present a fractional order Darcy law to describe fluid flow through porous media. The efficiency will be verified by investigating several groups of experimental data. The physical mechanism and parameter determination method of the new model are discussed.

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Continuum percolation of soft ellipsoidal pores in porous media

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ABSTRACT

Understanding percolation behaviors of pores is an open problem with great significance in the estimation of transport properties of porous media [1]. From a microscopic scale view, the pore structure as a complex network in a two-phase porous medium is normally viewed to be the random packing of soft particles with irregular geometry, in which a soft particle essentially represents a discrete pore with irregular geometry, as shown in Fig.1. A priori determination of continuum percolation in porous structures require detailed descriptions of important geometric and topological properties, such as pore size, shape and connectivity, which cannot be directly measured with available characterization techniques. So far, this research has only been performed numerically on spherical and cylindrical pores [2]. Yet, the assumption of perfect spherical or cylindrical pores is too idealistic to reflect the impact of morphologic details of pores in porous media. As a more suit approximation for pores with a realistic shape, soft ellipsoidal particles over a broad range of their aspect ratios ? such as spheres (? = 1), cylinders (? ? ?) and laminated flat plates (? ? 0) have been extensively applied to represent pores in the modeling study of porous media [3]. Here, we present a continuum percolation model of soft ellipsoidal pores by the Monte Carlo scheme. With the finite-size scaling method applied, the global percolation thresholds characterized by the critical volume fractions of ellipsoidal pores with different aspect ratios are measured. Comparing with the valid numerical results reported in the literature, the proposed continuum percolation scheme is confirmed with a favorable accuracy. In fact, the present model is an extension for the case of soft spheres introduced in the literature. While the accuracy and reliability of the proposed global percolation thresholds from the infinite domains are more superior to that of the local percolation thresholds of the limiting cases displayed in the literature. Furthermore, we find a quantitative mechanism between the global percolation threshold and the aspect ratio of ellipsoidal pores that the percolation threshold is decreasing function with the increase of aspect ratio of prolate ellipsoidal pores. It is very important that such a mechanism can be used as a theoretical criterion to allow researchers to further evaluate transport behaviors of porous media and particulate composites.

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Moment Lyapunov exponent and stochastic stability of a two degrees-of-freedom system under both harmonic and white noise excitations

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ABSTRACT

In this paper, the moment Lyapunov exponent and Lyapunov exponent of a two degrees-of-freedom system under both harmonic and white noise excitations are investigated. the moment Lyapunov exponent and Lyapunov exponent are important characteristics determining the stochastic stability of a dynamical system. The eigenvalue problem governing the moment Lyapunov exponent is established. Via the singular perturbation method, the second-order expansions of the moment Lyapunov exponent are obtained, which agree with the results obtained using Monte Carlo simulation well. The different cases when the system is in subharmonic resonance, combination additive resonance, and combined resonance in the absence of noise, respectively, are considered. Finally, the effects of the noise and frequency detuning on the stochastic stability of the system are discussed.

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Semi-analytical solutions for anomalous diffusion in 2D porous media via collocation Trefftz method

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ABSTRACT

Recent decade has witnessed a research boom on the meshless numerical fractional PDE techniques for anomalous diffusion in 2D porous media. The Collocation Trefftz method (CTM) is one of the most popular and powerful meshless methods, which is mathematically simple, and avoid troublesome mesh generation for high-dimensional problems involving irregular or moving boundary. This paper develops the CTM in conjunction with the recursive composite multiple reciprocity technique (RC-MRM) for numerical modeling of time fractional diffusion equations. It implements Laplace transform technique to obtain the corresponding time-independent inhomogeneous equation in Laplace space and then employs the CTM coupled with the RC-MRM to solve this Laplace-transformed problem. Unlike the other boundary discretization methods, the present method does not require any inner nodes, since the recursive composite multiple reciprocity technique (RC-MRM) is used to convert the inhomogeneous problem into the higher-order homogeneous problem. Finally, the Stehfest numerical inverse Laplace transform (NILT) is implemented to retrieve the numerical solutions of time fractional diffusion equations from the corresponding numerical solutions. Error analysis and numerical experiments demonstrate that the present CTM in conjunction with the RC-MRM is highly accurate and computationally efficient for time fractional diffusion equations to describe anomalous diffusion in 2D porous media.

Water flow across the land surface at various scales: Capturing anomalous dynamics using fractional operators

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ABSTRACT

Water flow across natural land surface can exhibit anomalous dynamics with apparent preferential and/or delayed flow pattern, due likely to the multi-scale physical heterogeneity embedded intrinsically in surface topography, soil hydraulic properties, land use, and vegetation coverage, among other factors that may not be measured exhaustively at all relevant scales. This study proposes a fractional-order continuity equation to quantify the scale-dependent anomalous behavior of overland flow, where spatiotemporally nonlocal terms built upon fractional derivatives are applied to capture the complex response of water flow to sub-grid heterogeneity. Physical model and process dynamics are also discussed for subsurface stormflow across hillslopes, a process showing similar anomalous behavior as surface runoff.

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Probing Osteocyte Pericellular Matrix and Its Roles in Bone's Mechanosensing

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ABSTRACT

A porous pericellular matrix (PCM) has been found to be present in the osteocyte lacunar-canalicular system (LCS) [1] and contain proteoglycan perlecan [2]. The osteocyte PCM has been hypothesized to modulate fluid shear stress [3] and amplify load-induced strain [4] experienced by the osteocytes and thus drive the bone remodeling process. However, quantitative measures of the pore size of the pericellular matrix and its alterations in vivo are lacking. For the past decade, we have developed a new method to quantify the osteocyte PCM by a combination of fluorescence recovery after photobleaching (FRAP) and mathematical modeling. Mice were injected with either a small or large fluorescent probe (sodium fluorescein, 376Da, 0.45nm Stokes radius; parvalbumin conjugated with AlexaFluor 488, 12kDa, 1.31nm Stokes radius) via tail vein [5]. After 0.5 or 3hr of circulation, paired FRAP tests were performed on the same lacunae while the freshly isolated tibia was subjected to 3N cyclic loading (1Hz) with 4 sec resting periods or to static loading (0.2N). The convective velocity for either tracer was calculated from the recorded transport enhancements of the FRAP tests [6]. The sieving coefficient of the osteocyte PC was thus obtained from the lag of the velocity of the large probe over that of the small probe (assumed to be the fluid velocity). Using a hydrodynamic model of the sieving effect of the fiber arrays to finite-sized probes [7], the effective edge-to-edge fiber spacing of the osteocyte PCM fibers was thus obtained to be 10.3, 13.4, 17.4 nm for 4-5 month-old B6 mice, 12-13 month-old B6 mice, and 12-13 month-old perlecan deficient mice, respectively [5]. The load-induced fluid flow shearing force and fluid drag force were estimated and agreed with in vivo experiment findings. Higher fiber density (smaller fiber spacing) is associated with higher fluid drag force and more robust bone formation under loading [5]. Perlecan's morphological (170nm long, 2-4 diameter) and mechanical properties (100pN breaking force, 500pN unfolding force, and 71MPa Young's modulus) detected by our single molecule force measurements with Atomic Force Microscopy support our hypothesis that perlecan tethers in the osteocyte PCM serves as flow sensor during bone's mechanosensing [8]. Understanding bone's mechanosensing mechanisms will help the development of effective treatments for osteoporosis, a significant health issue in our aging population.

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Experimental study of turbulence interactions across a permeable interface

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ABSTRACT

Many boundaries in engineering and environmental applications are oftentimes both rough and permeable, which, either in isolation or in combination, can significantly alter the flow characteristics compared to smooth and impermeable wall turbulence. Rough, impermeable wall turbulence has been studied for decades wherein topographic effects drive the turbulence in the near-wall region. Issues of wall permeability have also received considerable attention owing to the possibility of significant mass, momentum and energy transfer across the permeable interface. When these two boundary conditions occur together, as in many applications, they further complicate transport near the permeable interface, often leading to fundamental modification of the turbulence in both the free flow and the pore flow.

The present effort attempts to identify the individual roles of topography and permeability in wall turbulence. To this end, two physical wall models were considered in the current investigation: an impermeable rough wall composed of cubically-packed hemispheres (d = 25.4mm) and a permeable rough wall realized by cubically packing layers of uniform spheres and hemispheres (d = 25.4mm). Hence, the topographic effect on the free flow is identical in these two cases, allowing the role of permeability to be explored. An impermeable, smooth-wall case was also considered as a baseline reference for highlighting the effect of topography and permeability in the two other model scenarios. High-resolution particle image velocimetry (PIV) measurements were made for flow over each of the aforementioned wall conditions in the free flow for the impermeable cases, and in both the free flow and the pore space for the permeable model. Full optical access near the interface and within the pore space was achieved using a novel refractive-index matching (RIM) flow facility at the University of Notre Dame (Blois et al., 2012) whereby the wall models were fabricated of acrylic whose refractive index matched that of the working fluid in this facility (aqueous sodium iodide solution). Doing so minimized optical aberration and light reflection from the wall models, thus allowing PIV images to be successfully captured near the rough topography and across the permeable interface. The results from these experiments highlight the role of wall permeability in significantly modifying the turbulence characteristics in the near-wall region despite the mean streamwise velocity showing stronger sensitivity to the topographic effect. The pore flow shows strong correlation with the spatial arrangement of the permeable bed, with strong flow noted along pathways defined by the streamwise-aligned troughs of the cubic arrangement of the spheres.

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the slip driven-failure of liquid-infused porous media

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ABSTRACT

We study experimentally the failure of liquid-infused porous media under shear of external flows. Most of the previous work on this topic focuses on situations where the infused fluid is much more viscous than the external fluid thus the failure is mostly driven by the shear stress at the fluid-fluid interface. Here, we study the opposite limit: the viscosity of the infused fluid is much lower than that of the external fluid, hence it is the slip velocity at the interface that drives the infused liquid out. We systematically vary the flow rate and characterize both transient and steady-state responses. Our work could be employed to optimize the porous media to obtain higher liquid retention.

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Laminar drag reduction of a Newtonian fluid over random fibrous media

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ABSTRACT

The objective of this study is to examine velocity profile, shear stress, pressure distribution, and friction coefficeint over a specific fibrous porous media. In this study, we use experimental and numerical analysis to show that the drag force produced due to the laminar flow of a Newtonian fluid over a specific porous material lining a channel wall is considerably reduced. This concept, inspired by the almost frictionless movement of red blood cells through tiny capillaries, involves covering the planar surfaces with an array of porous media with permeability K and porosity ? [1-4].

Dynamic compression test was performed in order to choose a random fibrous material with the appropriate properties. Then, the properties of the fibrous material, i.e., its permeability K, the flexural rigidity, EI, and the maximum compression ratio were determined. The channel had a length of 90 cm, width of 50 mm, height of 30 mm, and PB fiber thickness of 4 mm. An interchangeable surface at the bottom wall has been coated with the PB fiber. Fig. 1a shows the measured velocity profile over smooth uncoated and polyester batting (PB) fiber-coated surface at Re=30. The velocity profile has been obtained using particle image velocimetry (PIV). An aqueous solution of 70% wt glycerin flows through the system. Fig. 1b shows the measured experimentally friction factor versus Reynolds number. The reduction in gradient of up to 26% is associated with the PB fiber-coated surface. We also compared our experimental data with the numerical predicted results. The solutions depend on the geometrical feature and the fiber interaction layer thickness ?=H/(K)1/2, where K is the fiber permeability and H is the fiber layer thickness. The resulting fits for measured and our numerical predictions of the velocity profile for PB fiber coated wall are excellent at ? =210. The fitted value of ? corresponds to K=3.6x10-10 m2. A reduction in gradient of up to 26% was associated with the PB fiber-coated surface. We have analyzed the experimental permeability of porous media from Darcy's law using volumetric flow rate per unit height and the pressure gradient. It was found that the estimated K differs from the fitted value by a factor of 10. The discrepancy between the two is to be expected due to deviations of the experiment from the model approximation such as flow steadiness and one-dimensionality. One of the implications of this analysis is that the analytical model suggests drag reduction is achieved when ? >100 in the porous medium regime.

Fig. 1. a) PIV measurements of the flow over PB fiber-coated surface at Re=30 and its comparison with smooth channel flow. b) Friction factor for smooth uncoated and PB fiber-coated surface as a function of the Reynolds number and its comparison with our numerical model. The scale bars have been deleted for simplicity.

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Macrodispersion induced by permeable surface topology

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ABSTRACT

Permeable and porous coated surfaces are common in natural and engineered systems and exhibit features that significantly deviate from their smooth impermeable counterparts. Even though flow and transport above such surfaces may be significantly affected by the surface topology, e.g. its porosity and permeability, the connection between the surface characteristics and their impact on macroscopic solute transport is still largely unknown. In this work, we focus on mass transport in a two-dimensional channel with permeable porous walls under fully developed laminar flow conditions. By means of perturbation
theory and asymptotic analysis, we derive both the set of upscaled equations describing mass transport in the coupled channel-porous matrix system and an analytical expression relating the dispersion coefficient and the surface properties, namely porosity and permeability. Our analysis shows that the impact of surface coatings topology on macrodispersion strongly depends on the magnitude of P$\acute{\mbox{e}}$clet number, i.e. on the interplay between diffusive and advective mass transport. The study provides a rigorous basis to relate matrix permeability to dispersion coefficient in coupled channel-matrix systems and gives quantitative guidelines for the design of porous/micro-patterned surfaces. The analysis also shows the possibility of controlling macrodispersion by either active (i.e. changing the operating conditions) or passive mechanisms (i.e. designing the pore geometry of the matrix) in the appropriate range of Peclet numbers. By elucidating the impact of matrix porosity and permeability on solute transport, our upscaled model lays the foundation for the improved understanding, control and design of microporous coatings with targeted macroscopic transport features. We validate our upscaled model by comparing concentration variation measured from experiments which performed on a series of microfluidic cells with different matrix geometries/permeabilities. Comparison shows a good agreement between our theoretical predictions and the experimental data.

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From Red Cells to Soft Porous Lubrication

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ABSTRACT

Biological scientists have wondered, since the motion of red cells was first observed in capillaries, how the highly flexible red cells can move with so little friction in tightly fitting microvessels without being damaged or undergoing hemolysis. Theoretical studies (Feng and Weinbaum, 2000; Wu et al., 2004) attributed this frictionless motion to the dramatically enhanced hydrodynamic lifting force generated inside the soft, porous, endothelial surface layer (ESL) covering the inner surfaces of our capillaries, as a red blood cell glides over it, Graph. 1. Herein we report the first experimental examination of this concept.

The experimental setup, Graph 2, consists of a running conveyer belt covered with a soft porous sheet, and a stationary instrumented inclined planar upper board. Twelve pressure transducers mounted on the upper board captured the pore pressure generation, while four load cells were used to capture the total lifting force, arising from both the pore pressure and the compression of the solid fibers. In addition, a load cell was mounted on the motor to measure the total friction force acting on the planing surface. One finds that the pore pressure distribution depends on the running belt velocity, U, the mechanical properties of the porous material, and the compression ratios of the porous layer. For a typical trial (h2/h1=5, h2/h0=1, U=3.325 m/s, where h2, h1, and h0 are the leading edge, trailing edge, and undeformed porous layer thicknesses, respectively), 73.9% of the lifting force was generated by the pore pressure (fair=73.9% in Graph.3, where fair denotes the relative contribution of the pore pressure to the total lifting pressure). With the increase of the U, fair increases and the friction coefficient between the fibrous porous layer and the planing surface decreases.

The experimental results were compared to the theoretical predictions by Feng and Weinbaum (2000) and Wu & Sun (2011), excellent agreement was observed. This finding, conclusively demonstrates the validity of the new lubrication theory for highly compressible porous media. This study has the potential to substantially improve our understanding of the behavior of highly compressible porous media as a lubricating layer with extraordinary potential for vastly increasing lift and reducing drag. From an energy efficiency and sustainability point of view, it has the potential of revolutionizing the design of lubricating bearings. In particular, it could lead to a new generation of soft lubricating bearings with far greater lift forces and much longer life. From the life science and health care point of view, it provides important insights for better understand the biophysics of the ESL which has been demonstrated to play an important role in cardiovascular systems. This work is supported by NSF CBET Grant #1511096.

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Investigation of a porous media model for blood flow in the choriocapillaris of the human eye

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ABSTRACT

Blood flow through the choriocapillaris provides nutrition to approximately the outer one third of the human retina, except in the foveal region in which the entire thickness is covered. It is believed that a detailed understanding
of this blood flow is important in assessing the causes/mechanisms, and possibly treating, ocular diseases (Zhu et al. [1]). Most previous studies have involved measurements, many of which are difficult, and even patient intrusive, in vivo. An exception is a recent contribution (Flower et al. [2]) in which an analytical model based on Darcy's law is considered in the context of a simple geometric model of the choroidal region. Solution of the corresponding equations provided blood-flow velocities consistent with measurements, but little physical detail could be produced.

In the present work, we employ computational fluid dynamics (CFD) to investigate a small portion of the region studied in [2] and focus on the relationship between porosity and shear stress (believed to contribute to visual pathologies) within the choriocapillaris. Simulations are performed
with a research code embodying the incompressible Navier-Stokes (NS) equations with Brinkman extension and Darcy and Forchheimer terms to permit calculations over the complete range of possible porosities. This code allows input of (spatially and temporally variable) porosity and permeability, use of the Kozeny-Carman formula, or application of a very general permeability model due to Tang and McDonough [3]. The numerical solution procedure employs standard methods for the NS equations, and current results are obtained with 0.005x0.025x0.025 mm resolution in the inlet/outlet and cross-flow directions,
respectively. Our initial calculations have qualitatively matched blood-flow speeds seen in physical measurements and have predicted shear stress with physically-reasonable amplitudes.

In the full-length paper we will provide results displaying the effects of porosity and permeability on velocity distributions and on shear stress, and we will address the question of whether a porous medium model is truly
appropriate for this situation. In particular, it is not clear that physically-correct shear stresses can be predicted with such a model.

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Interaction between turbulent free flow and pore space flow across the interface of a highly-permeable idealized bed

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ABSTRACT

Turbulent flow over an idealized porous gravel bed is investigated in the laboratory using particle image velocimetry (PIV) and refractive index matching (RIM) [1]. This combination allows for detailed examination of flow fields both in the near-bed region and within pore spaces. A packed bed comprising cubically packed spheres (diameter, D = 1.27 cm) was constructed. The permeability of the interface permits vertical momentum exchange between free stream and pore space flow. The mean flow field near the bed appears similar to that of skimming flow [2]. However, interactions between the subsurface and stream flow are apparent in instantaneous realizations. Figure 1 shows an example of distributions of instantaneous streamwise and wall-normal velocity V over and within the porous bed. Regions of high magnitude streamwise momentum near the bed correspond to downwelling into the pores, while low magnitude U correspond to upwelling from within the bed. During time periods when high momentum fluid is drawn from the stream into the subsurface, such as via a turbulent motion toward the bed, the streamwise momentum and velocity gradient near the bed increase. On the other hand, when relatively low momentum fluid is ejected from the subsurface, the streamwise momentum near the bed decreases. Thus, upwelling areas, whether instantaneous or enduring, experience low near-bed momentum, while downwelling areas experience high momentum. Overall, such motions across the bed interface serve as an important mechanism of vertical momentum exchange.

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InPore --- from a digitized rockstone to quantitative pore-scale porous media flow

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ABSTRACT

Fluid-filled porous media are ubiquitous in nature, science, and engineering. The performance of a porous media system relies on the movement of fluids, solutes, particles, electrical charges, and heat in pores. Traditionally, porous media flow is treated as a spatially and temporally averaged flow governed 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 me- dia. Recently, pore-scale porous media flow attracts more and more attention by utilizing newly developed radiological imaging techniques such as computed tomography (CT) thus the celebrated Navier-Stokes (NS) equations are solved for flow in pore spaces. 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 platform, named InPore, for pore-scale porous media flow[1] 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. InPore seamlessly integrates fully parallelized 3D image segmentation[4] and parallel acceleration of volumetric LBM[5] on CUDA platform to achieve extraordinary speed-up that other existing software and open source codes may not compete with. We

present an application study of natural gas/crude oil pore-scale flows in a digitized rockstone based on CT scanning image data. Focuses are on quantification of flow-rate and permeability in rockstones with varying porosity. The flow is driven by different pressure gradients. For given image data of a rockstone, we concurrently use InPore with smooth pore walls and binary pore structures plus LBM[6] to solve the pore scale flows. In the field of petroleum, it is common to segment the pore structure as a binary data, which is inaccurate. We evaluate the advantages and disadvantages of InPore for solving pore-scale porous media flow for its further development.

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Hydroelectric characterization of transport of suspended particles in a saturated porous medium:application of the method of self potential

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ABSTRACT

Clogging phenomena of the granular structure of oil reservoirs, infiltration basins, wells drilling and hydraulic bodies are the subject of several important research topics in different fields of engineering and industrial applications. This study is part of this framework, the main purpose is to provide a dual characterization hydroelectric approach to transport particles suspended in a saturated porous medium.
A campaign is conducted experiments in the laboratory; the tests consist in injections of kaolinite clay particles in columns filled with saturated sand.. In first step, different concentrations of the suspensions were injected at a constant flow rate in order to study the effect of the injection concentration, and at different flow velocities to study the influence of the latter. The hydrodynamic effects resulting from the damage of the porous media were investigated. In this work the sensitivity of the method of spontaneous potential (SP) was tested. The SP signal is correlated to the retention rate of injected particles and to changes in hydraulic head. The electrokinetic coupling coefficient has been studied at the spatial and temporal scale, its absolute value decreases with increasing the concentration of the injection solution. The effect of permeability, electrical conductivity and injection rate on apparent hydroelectric casting coefficient was studied.
The experimental study shows that the distribution of electrical signal has a complex origin electrokinetic, seismic, chemical, ... that can directly connect to the petrophysical properties of the porous medium.

Effect of biofilms on bed permeability

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ABSTRACT

Biofilms constitute an important form of bacterial life in aquatic environments and are present at the interface of fluids and solids, such as riverbeds or bridge columns. They are also utilized in bioreactors for bioremediation and water treatment purposes. Biofilms are permeable, heterogeneous, and deformable structures that can influence the flow and mass/momentum transport, yet their interaction with flow is not fully understood in part due to technical obstacles impeding quantitative experimental investigations. Recent studies have shown the profound effects of riverbed permeability on mass and momentum transfer. In alluvial rivers, bed porosity results in the generation of a diverse mosaic of ‘suction’ and ‘ejection’ events that are far removed from typical assumptions of turbulent flow structure over an impermeable bed [1,2].

This study represents a preliminary investigation on the interaction between flow and biofilms conducted in a closed water cannel facility (Figure 1) is a closed-loop water channel with 1×10 cm2 (H × W) cross-section and a 50-cm-long test-section with optical access from the top and side walls. Figure 2 presents the configuration where the channel is equipped with a 4-cm-deep permeable section consisting of cylinders normal to the bulk flow direction, forming a two-dimensional permeable bed. Prior to the flow experiments, the models are placed within an independent biofilm reactor to initiate and accurately control the biofilm growth. The models are then transferred to the water channel for water flow experiments at different biofilm growth stages. PIV measurements in this facility will be performed using a long-distance microscope to gain high image magnification and study flow over and inside the preamble bed.

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Shear-induced migration on red blood cells transport in the feto-placental vasculature system: consideration on oxygen transport

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ABSTRACT

The placenta is a transient vasculature organ, which enables nutrients and blood gases to be exchanged between the fetal and maternal circulations. Shear-induced migration of red blood cells (RBCs) is a well-known phenomenon characterizing blood flow in the small vessels (micrometer to millimeter size) of the vasculature system [1-4].

In this study, we consider the feto-placental vasculature system as a porous media and we model the extent of this migration in the feto-placental vasculature system as a particle-laden flows over porous medium ranging from micron to millimeter size of the vessels. RBC migration exerts its influence primarily on platelet concentration, oxygen transport and oxygen availability at the vessel surface, which could influence vessel wall disease processes. Using diffusive flux model [5], we model shear-induced particle migration to simulate the macroscopic behavior of the RBCs in a normal feto-placental vasculature system. Simulations show a migration of RBCs from the near-wall region with a lowering of wall haematocrit (volume fraction of RBCs) on the posterior side of the normal vessel and on the lateral external side of the vessels. The spatial and temporal patterns of wall haematocrit are correlated with the near-wall shear layer and with the secondary flows induced by the vessel curvature. In particular, secondary flows accentuate the initial lowering in RBC near-wall concentration in large vessles by convecting RBCs from the inner curvature side to the outer curvature side. The results reinforce data in literature showing a decrease in oxygen partial pressure on the inner curvature wall of the vasculature system induced by the presence of secondary flows. The lowering of wall haematocrit is postulated to induce a decrease in oxygen availability at the vessel surface through a diminished concentration of oxyhaemoglobin contributing with the reported lowered oxygen partial pressure to local hypoxia.

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Evaluation of groundwater available yield in the Pearl River Delta fault depression in South China

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ABSTRACT

The daily groundwater available yield is taken as the quantity of groundwater resources and the base for groundwater utilization. Taking a triangle area of the downstream West River in the Pearl River Delta in South China as the case study, this paper analysed the geological structure and fault zone distribution of the aquifer. The study area is located in the Pearl River Delta fault depression formed by the Xijiang major dislocations, the Guang-San foult and the Pearl River Estuary foult. Investigation of the hydrogeology features shows that the area is rich in karst water storage. One production well and three experiment wells, repectively numbered PW-1, CH1, CH2 and CH3, were used for pumping test. The test were lasted for 35 days with a stable water level at the 8th pumping day, while the water level recovered to the natural stage 7 days after the pumping stop with the stable pumping discharge 110 L/s, i.e, 396.47 m3/h or 9515.28 m3/d. Based on the pumping test data, the hydrogeological parameters including coefficients of transmissivity and percolation, elastic storativity, action radius and hydraulic slope were calculated. The annual mean groundwater resources of the study area was calculated to be 3127x103 m3/a or 8567 m3/d. The amount of groundwater replenishment of the study area which is computed to be 8567 m3/d and a little less than the test pumping discharge 9515 m3/d is taken as the available groundwater yield in the study area.

Pressure Infiltration Process for Synthesis of Graphene Reinforced Nano-Metal matrix Composites- A Review

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ABSTRACT

Metal-matrix composites (MMCs) offer noticeable advantages over traditional monolithic materials owing to their higher strength combined with lighter weight and are being used in sporting goods, automotive components, thermal management, and aerospace components. Recent research suggests that materials reinforced with nanoparticles, nanotubes and graphene can possess much higher physical, mechanical, and tribological properties than composites with much higher volume fractions of micro-size particles. Graphene as a nanomaterial has a high fracture strength of 125 GPa, making it an ideal reinforcement for MMCs. This study focuses on pressure infiltration processing of metal matrix nanocomposites reinforced with graphene.

Pressure Infiltration Processes are accepted and widely-used near-net shape production methods for manufacturing of MMCs. In pressure infiltration process, a preformed dispersed phase, i.e. a porous media (particulate, fibrous or woven ceramic or non-ceramic materials) is soaked in a molten matrix metal which fills the spaces between the dispersed reinforcement phases. The driving force of the infiltration process may either be the capillary pressure of the dispersed phase (spontaneous infiltration) or an external pressure applied to the liquid matrix phase (forced or pressure infiltration) using the vacuum-based, gaseous, mechanical, electromagnetic, centrifugal or ultrasonic techniques.

Despite the successful (albeit limited) demonstration of liquid-phase processing of metal-matrix nanocomposites, several processing challenges can be visualized. These include (1) difficulty in homogeneously dispersing nanoscale reinforcement; (2) extreme flocculation tendency of the nanoscale reinforcement; (3) increased viscosity (poor or inadequate fluidity) even at small loadings, due to large surface-to-volume ratio; (4) prohibitively large external pressures needed to initiate flow in nanoscale pores. This study is an attempt to address these issues and aim for novel techniques to produce graphene nano-metal matrix composites using the pressure infiltration method.

Keywords: Pressure Infiltration Processing, Graphene, Nanoscale, Metal Matrix Composites

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Influence of Fluvial Sedimentary Architecture on CO2 Trapping Processes in Deep Brine Reservoirs

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ABSTRACT

A number of important candidate CO2 storage reservoirs exhibit multi-scaled sedimentary architecture reflecting fluvial deposition, which influences the dynamics of injected CO2. Representing small-scale (cm to meter) features is critical to understanding capillary trapping processes, i.e. residual trapping (snap off) and capillary pinning (see Figure 1). The later mechanism may dominate in fluvial type reservoirs [1].
Recent studies have led to new conceptual and quantitative models for sedimentary architecture in fluvial deposits over a range of scales that are relevant to CO2 injection and storage. We used a geocellular modeling approach to represent this multi-scaled and hierarchical sedimentary architecture, and represented heterogeneity in all parameters, including heterogeneity in the saturation functions. With this model, we investigated the dynamics of CO2 plumes, during and after injection, in such reservoirs.
CO2 trapping and dissolution are profoundly impacted by the type of capillary pressure curve used, i.e. Brooks-Corey (with entry pressure) or van Genuchten (with no entry pressure). This difference is especially pronounced in heterogeneous reservoirs [2]. As a result, CO2 plume shape and position may be significantly different a long time after CO2 injection ceases (see Figure 2).
The detailed petrophysical and geological parameters of any specific reservoir are typically uncertain, which motivates studies of parameter sensitivity. Sensitivity analysis on the variability of basic parameters, such as contrast in permeability, irreducible water saturation, trapping saturation, and capillary entry pressure, will be presented.

Figure 1. a) Snap-off trapping. Counter-imbibition of brine (the wetting fluid) behind the advancing plume occurs preferentially through smaller pores and pore throats, trapping residual CO2 bubbles within the intervening pore bodies. b) Entry pressure pinning: CO2 is pinned below local contacts between an underlying rock type with larger pores (e.g. conglomerate cross-beds) and an overlying reservoir rock type with smaller pores and thus larger entry pressure (e.g. sandstone cross-beds). This occurs where the entry pressure of the finer-grained rock exceeds the buoyant pressure of CO2 in the coarser-grained rock.

Figure 2. Areal and vertical cross section of heterogeneous reservoir showing CO2 saturation after 10,000 days in case of van Genuchten (top panels) and Brooks-Corey (bottom panels) capillary pressure curves. In those simulations the snap-off trapping has been suppressed.

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Numerical Simulations of Water Penetration into Partially-saturated Sand

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ABSTRACT

Gravity driven water flow into an initially dry porous medium can lead to a non-monotonic behavior. Instead of a uniform flow front, water infiltrates in finger patterns, which has been observed experimentally [1, 3, 4]. Fingering effect cannot be described by the Richards equation or standard two-phase flow system, unless some additional terms are incorporated. One of the most effective approaches to model the observed saturation and pressure overshoot is to include the so-called non-equilibrium capillarity effect. Besides it, capillary or relative permeability hysteresis between imbibition and drainage processes also plays a key role in the degree of nonmonotonicity and its pattern.
In this work, we investigated and compared different approaches for modelling non-monotonic saturation and pressure behaviors in fingering effect. Either hysteresis and/or dynamic capillarity was included. We showed different overshoot patterns in various models and discussed the main regime of these numerical models. Moreover, we employed our model to fit the experimental data conducted by S. Fritz (2012) [2]. Five different combinations of dynamic and hysteretic effects were done to investigate our ability to simulate the experimental data.

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Experimental Capillary Desaturation Curve for Residual Nonwetting Phase in Natural Fractures

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ABSTRACT

The capillary number predicts residual-phase mobilization in porous media where capillarity causes the entrapment of a non-wetting phase. The entrapment occurs because of flow restriction and the surface tension between the displacing fluid and the fluid being displaced. Different forms of capillary number have been proposed for flow in porous media (Chatzis and Morrow, 1984). For flow in fracture, a capillary number was defined by (Hughes and Blunt, 2001). This definition uses only the mean aperture and the total width of the fracture to characterize trapping in the fracture.
Standing with a force balance on a trapped blob (Moore and Slobod, 1955). We propose a new definition of capillary number for fractures and perform laboratory experiments to define the capillary-desaturation curve using this definition. The "fractures" are made of glass plates, with a variety of degrees of roughness and correlation length of the roughness; these properties are included in our definition of the capillary number. The fracture surfaces where fully characterized and statistically analyzed. The fracture system was represented as a two-dimensional network of pore bodies connected by throats. The average hydraulic aperture of each fracture was measured in single-phase flow. Capillary desaturation curves were generated experimentally using water-air forced imbibition. The transparent nature of the system permits us to determine the residual air saturation from the captured images. Finally, the images were used to determine the saturation change over each incremental increased in pressure.
We show that the residual saturation-capillary number relationship obtained from different fractures, which vary in aperture width, roughness and correlation length, can be represented by a single curve. A definition of capillary number that does not account for roughness of the fractures does not correlate the data for different fractures. The experiments also show a relationship between the size of the trapped blobs and the glass roughness, which can be quantified using the correlation length of the roughness. Critical capillary number for the onset of mobilization of residual nonwetting phase in fracture was also determined.

The Effective Thermal Conductivity of Porous Media Predicted by Pore Size Distributions

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ABSTRACT

Several studies correlate the effective thermal conductivities with the porosity of porous media1–3. None of these studies, however, have investigated the effect of pore size and pore geometry on the effective thermal conductivity of the pore media. Considering the fact that micro-, meso-, and macro-pores have different heat and mass transfer characteristics, the prediction of effective properties of porous media can only be accurate and widely applicable if the prediction considers characteristics of all pores statistically4. Since porous media are composed of millions of pore, properties of porous media predicted by their pore size distributions (PSDs) are statistically significant. This study predicts the effective thermal conductivity of the porous medium using the statistical model based on the PSD, simulates the overall heat transfer properties of the porous media using a computational fluid dynamics (CFD) model, and compare the simulation results with experiments.

The effective thermal conductivity of a control volume made from two materials (the porous matrix and the filling material) is bracketed by the conductivity of two bulk materials (the volume fraction of the filling material equals the porosity) connect in parallel and the effective conductivity when these two materials connect in series5. The effective thermal conductivity in this study considers both the effect of pore size and the pore geometry through the PSD. The fundamental assumption in this study is that small pores are likely to be surrounded with spherical porous matrix and the effective thermal conductivity is equivalent to the thermal conductivity when the filling material (air) and the matrix material (glass) are connected in series. While large pores are likely to be generated by the hollow structure and its effective thermal conductivity is similar to the thermal conductivity when these two materials are connected in parallel6. The threshold diameter dthreshold in the statistical model that distinguishes connections in parallel and series is determined by experimental data.

This study also measures the effective thermal conductivity of home-made porous media made from 1 mm and 5 mm glass beads and the porosity of these porous media, ?, are measured to be 0.41. The PSDs in porous media, which can be measured by pore size analyzers, typically follow log-normal distributions. The statistical model in this study estimates that mean pore sizes of the log-normal distributions (with the shape factor of 0.45) are 0.6 mm and 3.25 mm, respectively, to obtain the same surface area per volume with porous media made from 1 mm and 5 mm glass beads. The predicted thermal conductivities of porous media and the simulated transient temperature distributions in the porous medium are compared with experimental measurements to find out the threshold pore sizes. Since the characteristics of the geometries can be quantified by the PSD of the porous medium, this theory to predict the effective thermal conductivity can be conveniently applied to other porous media with different geometries, such as metal foams.

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On the diagnosis of transport processes by means of single and multiple clocks

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ABSTRACT

The concepts of age and travel time are widely used to quantify the transport rate of tracers or contaminants in the environment, as well as to making estimates on pore velocity magnitudes. Water age (the relative time taken by water molecules since they entered the reservoir of interest) has today become a quantity of specific interest for it can be associated to a perfect conservative tracer which can be assessed by means of field measurements and lab analysis as well as by mathematical and numerical modelling. Age is subject to both advection and dispersion/diffusion processes, and relates only to the time taken to reach a given location while disregarding other aspects of the path followed by water of by a tracer parcel. Lifetime expectancy is this complementary travel time that focuses on the time remaining at a given location prior to exiting the domain. To keep track of the subregions visited by the tracer parcel, ages and lifetime expectancies can be partitioned in a composite way so that they are able to relate to the times spent (or still to be spent) in the different subregions of the reservoir. Such composite (or partial) travel times can be computed in an Eulerian framework very similar to that used to assess the global quantities.
A series of theoretical and practical examples are used to demonstrate the versatility of the concept of travel times (and their decomposition) and the potential new insights that can be gained with it. Targeted fields of application range from subsurface, overland and oceanic contexts, to industrial use of artificial porous media.

Thermodynamics of fluid interfaces in pores

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ABSTRACT

The equilibrium shape of a liquid–vapor interface inside a solid pore effects many porous media phenomena. Pore microscale and nanoscale confinement and the resulting curvature of the liquid–vapor interface can suppress or enhance phase transitions (capillary condensation, capillary evaporation). The equilibrium behavior is also a key determinant in kinetic phenomena such as nucleation of a new phase, evaporation, condensation and flow. Gibbsian composite-system thermodynamics [1] gives a framework to predict equilibrium interface behavior inside pores [2-5]. The Gibbsian approach involves: i) deriving the conditions for equilibrium, ii) combining the conditions for equilibrium with equations of state for the phases and solving the resulting set of equations to get equilibrium sates, iii) determining what function acts as the thermodynamic potential for the system, and iv) examining the maxima and minima in the thermodynamic potential to understand the stability of the equilibrium states, thus determining the system behavior. We have applied Gibbsian composite-system thermodynamic stability analysis to understand in a cross-geometry way, several interesting phenomena for fluid interfaces in pores including critical behavior of a fluid confined in a nanoscale pore far from the critical point [3] and the suppression or enhancement of new phase nucleation (liquid from vapor or vapor from liquid) inside nanoscale gaps in the sphere–plate, plate–plate and conical pore geometries [4,5]. The relationship of fluid meniscus height to pore diameter will also be discussed. This research was funded by the Natural Sciences and Engineering Research Council (NSERC) of Canada. J. A. W. Elliott holds a Canada Research Chair in Thermodynamics.

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Self-similar viscous gravity currents in heterogeneous porous media: Second-kind solutions

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ABSTRACT

We summarize our recent combined experimental-theoretical-computational study of the effects of horizontal heterogeneities on the propagation of viscous gravity currents with applications to porous media flows. Our model geometry is a horizontal channel (specifically, a Hele-Shaw cell) with variable gap thickness in the streamwise direction in the form of a power law. We demonstrate that two types of self-similar behaviors emerge as a result of such horizontal heterogeneity: (a) a "first-kind" solution is found using dimensional analysis for currents that propagate away from the origin (a point of zero permeability); (b) a "second-kind" solution is found using a phase-plane analysis for viscous gravity currents that propagate toward the origin. Using the phase-plane formalism, we are able to construct the universal second-kind self-similar current shape. Additionally, still employing self-similar intermediate asymptotics and the phase-plane formalism, we identify self-similar behaviors in the "post-closure" regime, i.e., once the current reaches the geometric origin and begins to fill the model porous medium. The theoretical predictions show good agreement with lab-scale experiments using Hele-Shaw cells and also numerical solutions of the governing partial differential equation developed under the lubrication approximation.

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Analytical models of hysteresis in multiphase phenomena in porous media

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ABSTRACT

Multiphase phenomena in porous media exhibit hysteresis in continuum-scale variables such as capillary pressure and relative permeability, but it is at the pore-scale where hysteresis originates. Therefore, continuum models of hysteresis must in some way capture the effects of the distribution of fluid phases within pore space. This is often accomplished with simulations of various types carried out on pore networks. Here, we present analytical models of hysteresis that relate the collective effect of microscopic physical processes to macroscopic changes using percolation theory or by statistical arguments. In an analysis of hysteresis in quasisteady drainage and imbibition, we find it useful to consider the statistics of displacement of fluid-fluid interfaces to model the ink-bottle effect. As the capillary pressure is varied slightly from equilibrium, a small fraction of the interfaces will move down the pores until they come to a stop. The displacement of each moving interface is described by a Poisson process, and is dependent on the pore-size distribution of the porous medium. This relates changes in saturation to changes in capillary pressure, and leads to hysteresis naturally when the direction of change in capillary pressure is reversed.

Three-dimensional Pore Scale Imaging of Trapped Supercritical Carbon Dioxide in a Mixed-wet Carbonate

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ABSTRACT

Depleted oil reservoirs are perceived as initial project opportunities for carbon storage when coupled with CO2 enhanced oil recovery (EOR). With absent strong climate policy, the incremental oil recovery from EOR provide a significant revenue stream and makes CCS economically attractive. Capillary trapping has been identified as a key storage process that leads to the immobilization of CO2 as a non-wetting droplets surrounded by brine in the water-wet porous rocks of saline aquifers, limiting the extent of plume migration, enhancing the security and capacity of CO2 storage. In contrast, carbonate oil reservoirs are characterized by a mixed-wet state in which the capillary trapping of nonpolar fluids have been observed to be significantly reduced relative to trapping in water-wet rocks typical of saline aquifers unaltered by the presence of hydrocarbons. There are, however, no observations characterizing the extent of capillary trapping that will take place with CO2 in mixed-wet rocks. We use X-ray microtomography, at a resolution of 5 ?m, to investigate the pore-scale arrangement of supercritical CO2 droplets in situ in water-wet and mixed-wet carbonates at temperatures and pressures representative of subsurface oil reservoirs and saline aquifers. The measurements were made while maintaining chemical equilibrium between the fluids (CO2 and brine) and rock phases to prevent reaction with the core sample and replicate conditions far away from the injection site. The measurements were also compared with trapping of N2 to test the validity of using analogue fluids to replicate CO2 trapping in mixed-wet systems. Here we show that residual CO2 trapping of supercritical CO2 in a limestone altered to a mixed-wet state with oil is significantly less than trapping in water-wet systems characteristic of saline aquifers. The measurements were made on Estaillades limestone core samples. It was made on its original water-wet state and after altering the wetting properties with crude oil to a mixed-wet system. We anticipate this work to highlight a key issue for the early deployment of carbon storage – that those sites which are economically most appealing as initial project opportunities are the very locations in which the contribution of capillary trapping to storage security will be minimized. This should serve as a starting point for modelling studies to incorporate the reduced impact of capillary trapping on CO2 injection projects using hydrocarbon reservoirs.

On a new statistical approach for homogenization of random heterogeneous and polydiffusive random porous materials

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ABSTRACT

Assessing the effective diffusion coefficient of complex heterogeneous materials still remains an unresolved subject. Very few homogenization schemes are able to predict them for a wide range of materials. Moreover, they fail reproducing the evolution of the diffusion coefficients while the materials are subject to degradations. This is especially the case for cementitious materials, whose pore structures expand over a wide range of pore sizes. The morphology of the macroporosity is determinant for estimating the overall properties, but no laws are able to include such features.

As diffusion is a random process, a new homogenization schemes, based on a statistical description of diffusion at the pore scale, is obtained. The latter is based on geometric concepts such as chord-length-distributions. A wide range of microstructures are tested and confronted to diffusion coefficients obtained from a random-walk algorithm. We show that this new scheme actually is able to reproduce simulated values for very different morphologies of porosity. These microstructures generally contain two diffusive phases, presenting a high diffusivity contrast, and some other non-diffusive phases.

Though it does not depend on any percolation threshold, we also show that this modelling is very sensitive to connectivity and percolation, as well as on small variations of overall porosity. This is possible thanks to the definition of a new concept : the hyper-chord-length-distribution of a phase.

Method for determining REV and ranking rock heterogeneity based on local permeability and porosity

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ABSTRACT

We detail a novel method to determine the degree of rock heterogeneity based on its permeability and porosity. We use binerized 3D images obtained using micro-CT. These images are subdivide into N_i-slices where i = {x, y, z} along the three spatial coordinates. This is illustrated for the z-direction in figure 1. For every slice we calculate the porosity and the permeability using a single-phase Lattice Boltzmann method with the Multiple-Relaxation-Time model. The fluid viscosity and the pressure gradient across a slice in the flow direction are assumed to be constant. It is found that the obtained permeability data set is typically log-normally distributed whilst the porosity is normally distributed. We define the fluid Net Throughput as NT_ij=k_ij/(\phi_ij [\chi \Delta N_j]^2), which is the ratio of the volumetric throughput obtained from Darcy's equation to the void space of a slice of a porous medium. This is essentially a dimensionless form of the interstitial velocity. In here, k_ij and \phi_ij are respectively the permeability and porosity of the j-th slice in i-th direction. Furthermore, \Delta N_j is the thickness of the j-th slice in [voxels] and \chi the voxel size in [m/voxel]. We compute the Coefficient of Variation (CV = standard deviation / arithmetic mean) of NT_ij as a function of the slice thickness. CV is a measure for the dispersivity of NT_ij and it reaches a peak at a given slice thickness which we define as the critical length in the i-th direction. The critical lengths in the x, y and z directions forms a Representative Volume Element (REV) taking into consideration both permeability and porosity of a rock. We also show how one can determine the REV in case the scanned rock sample is smaller than the REV. To demonstrate this approach we examine three type of rocks: (1) Bentheimer, (2) Clashach, and (3) Estaillades. We found that Estaillades sample is most anisotropic and heterogeneous. Our Clashach sample is more heterogeneous, but less anisotropic than Bentheimer. Finally, we show that our slicing method can be readily used to compute spatial statistics [1]. The semi-variance of the log permeability fits the spherical model and the range obtain from variograms [2] can be used to construct a REV based on permeability only. We compare this REV with the one obtained using the Net Throughput approach and found that porosity plays a significant role in determining a Representative Volume Element.

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Simultaneous measurement of macroscopic strain and mesopore deformation of silicas with hierarchical porosity

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ABSTRACT

Monolithic silica with hierarchical porosity are excellent model systems for studying adsorption-induced deformation, both on the micro- and macroscale. Using a specially designed sample cell we investigated such silica monoliths in terms of sorption-induced deformation simultaneously with respect to their macroscopic strain as well as the deformation of their strut substructure defined by hexagonally ordered cylindrical mesopores with pore diameter < 10 nm (Figure 1, left image).
We used water adsorption at 290 K for the experiments. To prevent changes of the silica porosity during analysis we aged the samples under humid atmosphere prior to the measurements. The sample cell was designed to allow neutron scattering and simultaneous dilatometric monitoring of the sample. Humidity in the air tight cell was stepwise increased by connecting the cell to a dosing unit. To provide unequivocal information on changes of the microstructure, partially deuterated water was used as adsorbate in the experiment; as a consequence the adsorbate was invisible to the neutrons and the resulting scattering from the hexagonal array of mesopores was just affected by the changes the silica microstructure during sorption. In separate experiments nitrogen sorption and water isotherms were recorded.
We investigated three different types of silica samples: one derived from supercritical drying and subsequent aging, the second being additionally calcined, thus creating well accessible microporosity and the third with significantly lower microporosity due to heat treatment of the supercritically dried sample at 750 °C for 15 min. The meso- and macroporosity is almost not affected by the different post-treatments (sintering at 750°C only reveals a 10 % decrease of the mesopore diameter, see Figure 1, right image).
In all samples the deformation is dominated by Bangham's effect [1]; accordingly, monotonous expansion is observed. While the macroscopic strain reveals a max. expansion < 0.1 %, the scattering peak related to the hexagonal array of mesopores shows an asymmetric shift (with the low q wing shifting by about 6%) indicating that there is no homological expansion of the dry mesopore system when humidity is increased. We provide a first approach to model the scattering curves and relate the findings to the macroscopic strain of the samples. In particular we discuss the impact of different surface groups and microporosity on sorption induced deformation.

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Porous media for light gas isotope separation

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ABSTRACT

Separating gaseous mixtures that consist of very similar particles (such as mixture of light gas isotopes or mixtures of noble gases) is one of the challenges in modern separation technology. Especially D2/H2 separation is a difficult task since its size, shape and thermodynamic properties share each other. Recently, confined space of porous media has received increased attention as an efficient method for hydrogen isotope separation, and this is so-called quantum sieving[1]. Despite many theoretical calculations[2], however, it has been difficult to identify a feasible microporous material up to now. Among various porous materials, the novel class of microporous framework materials (COFs, ZIFs and MOFs) is considered as the most promising approach for isotope sieving due to ultra-high porosity and uniform pore size which can be tailored in these materials.
In the work, we focused on the investigation of the fundamental correlation between D2/H2 molar ratio and pore size at optimized operating conditions by using different nanoporous frameworks. It reveals that the D2/H2 molar ratio is strongly depending on pore size, pressure and temperature. The smaller pore size and the lower P, T, the higher separation factor can be obtained[3]. Afterwards, two strategies for satisfying industrial requirements are introduced. Firstly, one way of increasing the operating pressure is presented by using cryogenically flexible COFs[4]. Secondly, a different chemical affinity of isotopes on strong adsorption sites is demonstrated in order to increase the operating temperature for isotope separation[5]. Finally, deuterium separation from a diluted isotope mixture is experimentally demonstrated by applying a temperature swing process.

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A hydromechanic-electrokinetic model for monitoring CO2 geosequestration

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ABSTRACT

A computational model for monitoring CO2 flow in a deformable fractured porous medium using the electrokinetic front tracing technique is introduced. The governing field equations are derived based on the averaging theory and solved numerically based on a mixed finite element discretization scheme [1-3]. The standard Galerkin finite element method is utilized to discretize the deformation and the diffusive dominant field equations, and the extended finite element method, together with the level-set method, is utilized to discretize the advective dominant field equations. The level-set method is employed to trace the CO2 plume front, and the extended finite element method is employed to model the high gradient in the saturation field front. This mixed discretization scheme leads to a convergent system, giving a stable and effectively mesh-independent model. Effects of the salinity content on the streaming potential are discussed.

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Multi-scale imaging and elastic simulation of carbonates

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ABSTRACT

Digital Rock Physics (DRP) is an emerging technology that can be used to generate high quality, fast and cost effective special core analysis (SCAL) properties compared to conventional experimental techniques and modeling techniques. The primary workflow of DRP conssits of three elements: 1) image the rock sample using high resolution 3D scanning techniques (e.g. micro CT, FIB/SEM), 2) process and digitize the images by segmenting the pore and matrix phases 3) simulate the desired physical properties of the rocks such as elastic moduli and velocities of wave propagation.

A Finite Element Method based algorithm, that discretizes the basic Hooke's Law equation of linear elasticity and solves it numerically using a fast conjugate gradient solver, developed by Garboczi and Day [1] is used for mechanical and elastic property simulations. This elastic algorithm works directly on the digital images by treating each pixel as an element. The images are assumed to have periodic constant-strain boundary condition. The bulk and shear moduli of the different phases are required inputs. For standard 1.5" diameter cores however the Micro-CT scanning resolution (around 40 µm) does not reveal smaller micro- and nano- pores beyond the resolution. This results in an unresolved "microporous" phase, the moduli of which is uncertain. Knackstedt et al. [2] assigned effective elastic moduli to the microporous phase based on self-consistent theory (which gives good estimation of velocities for well cemented granular media). Jouini et al. [3] segmented the core plug CT scan image into three phases and assumed that micro porous phase is represented by a sub-extracted micro plug (which too was scanned using Micro-CT). Currently the elastic numerical simulations based on CT-images alone largely overpredict the bulk, shear and Young's modulus when compared to laboratory acoustic tests of the same rocks. For greater accuracy of numerical simulation prediction, better estimates of moduli inputs for this current unresolved phase is important. In this work we take a multi-scale imaging approach by first extracting a smaller 0.5" core and scanning at 13 µm, then further extracting a 5mm diameter core scanned at 5 µm. From this last scale, region of interests (containing unresolved areas) are identified for scanning at higher resolutions using Focalised Ion Beam (FIB/SEM) scanning technique reaching 50 nm resolution. Numerical simulation is run on such a small unresolved section to obtain a better estimate of the effective moduli which is then used as input for simulations performed using CT-images. Results are compared with experimental acoustic test moduli obtained also at two scales: 1.5" and 0.5" diameter cores.

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A particle-based computational method to determine capillary pressure - saturation curves in porous media

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ABSTRACT

Wicking of liquids in absorbent porous media is driven by capillary forces. The level of saturation of the porous structure influences the magnitude of the capillary forces. This work presents a novel particle-based computational method to determine capillary pressure vs saturation behavior of fibrous porous media. Both liquid and gas are represented by coarse-grained particles. Additionally, the liquid particles display a soft, density–dependent repulsion that prevents any extended structuring of the liquid. The particle models are parameterized against analytical results obtained using the Young-Laplace equation in straight capillary tubes. Subsequently, the static capillary pressure is obtained a function of saturation for fibrous porous media. In accordance with known experimental results, significant hysteresis in imbibition and drainage directions is obtained. The method is also applicable to other types of porous media

New solutions for image-based porous media analysis & simulation

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ABSTRACT

The analysis of 3D image data (as obtained from CT, Ultrasound, micro-CT, FIB-SEM etc.) for porous media applications is typically limited to visualization and measurements. Finite Element (FE) simulation is a very powerful tool that allows researchers to simulate physical phenomena such as fluid flow through and/or mechanical deformation of porous media. Linking 3D image data to FE simulation has traditionally been a slow process largely due to the technical difficulty and the labor intensive process of converting 3D images into robust, efficient and accurate volumetric FE meshes for simulation. A typical workflow may include, for example, STL-based FE meshing, which is a very inefficient and labor intensive method.

New tools have been developed for generating FE models from 3D image data of porous materials that solve these challenges through direct image based meshing [Young et al. 2008]. Techniques for visualization, measurement and simulation of porous media will be discussed, as will how advances in both imaging and computing power are making it straightforward to acquire qualitative and quantitative information from porous media samples through FE simulation. Methods have also been implemented in software for calculating effective material properties from scanned samples using FE-based homogenization; this has applications to characterizing absolute permeability, and to broader analysis of properties such as elasticity and electrical conductivity.

An example of how these techniques can be used will be given from work carried out by Micro Photonics Inc. (Allentown, PA), Simpleware Ltd. (Exeter, UK) and Device Analytics (San Diego, CA). The presentation will outline the steps taken to obtain image data of a porous filter prior to generating a 3D image-based FE mesh suitable for carrying out flow simulations. The many pitfalls and successes of this workflow will be discussed, with the goal of elucidating best practices to avoid typical roadblocks and errors in this new, rapidly expanding and cutting edge field of 3D image-based simulation.

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An Advanced Reservoir Simulator for Tracer Transport in Multicomponent Multiphase Compositional Flow and Applications to the Cranfield CO2 Sequestration Site

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ABSTRACT

Reservoir simulators are widely used to constrain uncertainty in the petrophysical properties of subsurface formations by matching the history of injection and production data. However, such measurements may be insufficient to uniquely characterize reservoir's properties. 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. Oak Ridge National Laboratory has been piloting this technology during and following three CO2 injection campaigns at the Cranfield, Mississippi, CO2 sequestration test site. Multiple perfluorocarbon tracers and isotopes were injected together with CO2 and monitored at two wells at 68 m and 112 m from the injection site. 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 the CO2 plume did not expand radially, but that multiple flow paths developed towards the monitoring wells. This is indicative of either channeling through high permeability pathways or of fingering. The results demonstrate that tracers provide an important complement to transient pressure data. To aid the development of this new technology, we enhanced a fully compositional multiphase reservoir simulator to interpret tracer transport. Our research simulator uses higher-order finite element methods that can capture the small-scale onset of fingering on the coarse grids required for field-scale modeling, and allows for unstructured grids and anisotropic heterogeneous permeability fields. Mass transfer between fluid phases and phase behavior are modeled with rigorous equation-of-state based phase-split calculations. We present our tracer simulator and preliminary results related to the Cranfield tracer experiments.

Heterogeneous charged porous media and non-linear electrokinetic effects

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ABSTRACT

The heterogeneous charged porous 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 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 Model (METLM) 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 strengthened by imposing pH or concentration gradient. Third, the heterogeneous charged pores may impose strong local non-linear electrokinetic phenomenon which would influence 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 METLM 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 reproduction of microstructures of porous media.

A novel microfluidic framework introduced for low capillary number moving interface

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ABSTRACT

Micro-droplet formation and mobilization is an emerging area of research due to its wide-ranging usage within microfluidics application relevant to tight porous media (Andrew et al., 2015). Physical understanding of this process at the pore scale is helpful in exploring macroscopic phenomena in oil and gas recovery and also forms the basis of many potential applications such as synthesis of new materials, formulation of products in pharmaceutical, cosmetics and food industries. The standard two-phase Volume Of Fluid (VOF) and/or Level Set (LS) methods for interface tracking between two immiscible fluids, have been used extensively in the literature to perform numerical simulations of droplet break up/formation in porous media (Wörner, 2012). These methods are less successful for the study of phenomena when the combined effect of viscous and capillary forces is dominant. This is mainly due to difficulties in predicting the flow in presence of high capillary forces encountered in flows at the pore scale, which can introduce non-physical (parasitic) velocities or instabilities in the numerical results. In the present work, a novel dynamic VOF-based framework for reducing parasitic velocities at low capillary number flows (based in the works (Georgoulas et al., 2015; Raeini et al., 2015) work, as well as an improved Coupled LS-VOF (CLSVOF) method for conservative sharp interface tracking, are introduced. These frameworks are compared with the commonly used for the prediction of relaxation of static droplets with varying sizes and they are also utilized to study the dynamics of oil droplet trapping and mobilization within pore throats through a T-junction configuration. The overall numerical model development has been conducted within the open-source, CFD Toolbox, OpenFOAM (version 2.3.x). The Navier–Stokes equations are discretized using a finite volume approach, while the Volume Of Fluid method is used to capture the location of interfaces. The olume fraction (alpha) is advected implicitly and additional algorithms for compressing, sharpening and smoothing the interface are implemented in order to guarantee its physical thickness and curvature. Surface tension forces are then computed based on the sharp/smooth (alpha) field which maintains a steep transition area for capillary pressure. The influence of the static/equilibrium contact angle imposed at the rigid wall is also considered in order to account for various wettability effects. The developed numerical method targets efficient modelling of multiphase flows in the micro-scale with complex interface motion and irregular solid boundaries. It allows correcting surface forces and permits simulations at low capillary numbers dampening out non-physical velocities. Moreover, the addition of the adaptive grid refinement method and the implicit formulation for the equation of volume fraction, allows larger time steps and thus lower computational cost. Overall, the comparison of computational results with analytical models and experiments shows that the introduced framework improves the accuracy of the original VOF method when the surface tension influence is predominant. Some indicative results for a static droplet case (150 micron) are depicted in Figures 1 and 2 below.

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Grid flexible numerical methods for poro-elasticity applied to geological models using virtual element and mimetic finite difference

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ABSTRACT

Compact representations of geological models naturally lead to polyhedral grids due to the physical processes of sedimentation, errosion and faulting. We investigate couplings between methods which work on polyhedral grids for linear mechanics and finite volume based methods for flow, which remain
the standard methods used to simulate multiphase flow. For linear elasticity we consider the virtual element method while for the flow, we consider Mimetic Finite difference. In particular we investigate the behaviour of the methods for distorted faulted grids with high aspect ratios which is common in subsurface flow problems. The methods can handle general linear elasticity parameters and general permeabilities. We study the accuracy of the method in the evaluation of stress in view of future applications to fracturing criteria. We will demonstrate how the flexibility with regards to the grid can be exploited to avoid numerical artifacts.

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Parallelized Finite Element Simulator for Fully Compositional and Black Oil Flow on Unstructured 3D Grids: A Scalable Hybrid MPI/OpenMP Model

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ABSTRACT

We present a hybrid parallel simulator for reservoir engineering problems of the highest complexity: fully compositional and black oil, three-phase, compressible flow on any type of 3D unstructured grid. When applicable, the model is reduced to a black oil description to increase computational efficiency; we compare the accuracy of black oil model in addition to its speed-up with those of fully compositional model.

In the context of black oil modeling, where hydrocarbon components are divided/lumped into a gas and an oil component with only gas component being allowed to transfer between oil and gas phases, study cases may involve treating a variable bubble point pressure (Pb) throughout the reservoir (e.g. in water flooding into saturated reservoirs, or introducing gas into an undersaturated grid cell). Traditionally, a primary variable switching strategy for phase appearance/disappearance has been proposed, which inherits convergence and phase identification issues – beside using low order numerical schemes. However, we adopt an overall molar composition-based framework that can self-consistently take care of such complication. Specifically, we compute the black oil properties from tables constructed as a priori by means of fully compositional phase-split calculations in an initialization step. Phase properties across a broad range of pressures versus the composition of black oil pseudo-components are interpolated to correctly model the transitions between saturated and under-saturated states of different Pb. While preserving the accuracy, we could gain considerable speedup in black oil model – more pronounced in cases of 3D and saturated reservoirs.

Finite element (FE) methods are adopted that are well suited to parallelization and provide maximum flexibility in discretizing the geometry. Mass transport is updated explicitly by a locally mass conserving and readily parallelizable discontinuous Galerkin method. Phase split computations consume the bulk of CPU time, but these are local and trivially parallelized. Globally continuous pressure and velocity fields are obtained through an implicit mixed hybrid FE update, which result in a non-trivial parallelization problem involving domain decomposition. High-performance parallel algebraic multigrid preconditioners and solvers for large, sparse linear systems have been implemented. In particular, BoomerAMG preconditioner (threaded in the solve/smoothing phase), Hypre, and PETSc libraries for preconditioners/solvers are tested. A high level of parallelization is achieved through mixed message-passing/threaded programming to benefit from clusters of SMPs by both intra- and inter-node parallelization. Pure OpenMP and pure MPI on shared and distributed memory systems, respectively, are also investigated to determine which architecture can achieve the minimal parallelization overhead depending on the problem size. The robustness, accuracy, and scalability of our parallel FE simulator are demonstrated for several complex problems where we have attained Super-linear speedup in phase-split computations so far.

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Two-component two-phase reduced numerical model for methane hydrate formation under conditions of variable salinity. Time-stepping variants and sensitivity.

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ABSTRACT

Computational models of multiphase multicomponent flow and transport in subsurface have several challenging components including discretization in space and time as well as accounting for phase equilibria. The crucial variables include the reservoir and fluid pressures, temperature, and mixture concentrations. In this paper following [3] we consider a reduced computational model of methane hydrate formation in variable salinity conditions which accounts for concentrations of methane and of salt in liquid and hydrate phases. We give details on the discretization and phase equilibria implementation.

Methane hydrate, an ice-like compound, is found in favorable subsurface conditions under the ocean floor and in the Arctic. For its evolution we consider a reduced model in which we assume that the pressure is predominantly hydrostatic and temperature follows the geothermal gradient. These assumptions are commonly made for modeling the hydrate formation and dissociation. We propose a reduced thermodynamic model adapted to a case study from Ulleung Basin, and we implement it as part of the phase equilibria package in our numerical model. The main advantage of our model and implementation over fully imlicit fully comprehehsive models is that they allow to introduce several robust time-stepping variants: Implicit, Semi-implicit, and Sequential. The reduced model also allows various rigorous mathematical analyses; see our work in [1,2] where we considered a simplified version of the current model in which salinity was fixed. In the presentation we compare the accuracy and efficiency of these variants depending on the spatial and temporal discretization parameters. We also study sensitivity of the model to the simulation parameters and in particular to the reduced phase equilibria model.

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Three-Dimensional Pore-scale Simulation of Root-Soil-Groundwater Interaction

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ABSTRACT

Root water uptake and hydraulic redistribution are important mechanisms in the vegetated soil systems. However, due to the complex structure of the plant roots and heterogeneity of the soil, computational simulations of such interactive systems become challenging. The objective of the current research is to apply a three-dimensional pore-scale approach to study root-soil-groundwater interaction and its impact on the hydrodynamic transport parameterization at the plant scale. A 3D X-ray computational tomography (XCT) was used to capture the structure of a plant root. Computational fluid dynamics (CFD) techniques were then used to numerically simulate the root-soil-groundwater system. The plant root conductivity, soil hydraulic conductivity and transpiration rate were shown to control the groundwater distribution. The flow variability and soil water distributions in different case scenarios were investigated. Parameterizations under multiple grid resolutions were processed to show their impacts on the average conductivity. The current approach provides realistic simulations in such ecosystems with useful information directly linked to upscaled models.

Numerical Study of Groundwater Flow Cycling Controlled by Seawater/Freshwater Interaction in a Coastal Karst Aquifer through Conduit Network Using CFPv2

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ABSTRACT

A groundwater flow cycling in a karst springshed and an interaction between two springs through a subground conduit network are numerically simulated using CFPv2, the latest research version of MODFLOW-CFP (Conduit Flow Process). Spring Creek Springs and Wakulla Springs, located in a marine estuary and 11 miles inland, respectively, are two major groundwater discharge spots in the Woodville Karst Plain (WKP), North Florida, USA. A three-phase conceptual model of groundwater flow cycling between the two springs and surface water recharge from a major surface creek (Lost Creek) was proposed in different rainfall conditions. Tracer tests and cave diving found a high permeable subground karst conduit network connecting the two springs. Flow rate of discharge, salinity, sea level and tide height at Spring Creek Springs could significantly affect groundwater discharge and water stage at Wakulla Springs simultaneously.
Based on the conceptual model, a numerical hybrid discrete-continuum groundwater flow model is developed using CFPv2 and calibrated by field measurements. Non-laminar flows in conduits and flow exchange between conduits and porous medium are implemented in the hybrid coupling numerical model. Time-variable salinity and equivalent freshwater head boundary conditions at the submarine spring as well as changing recharges have significant impacts on seawater/freshwater interaction and springs' discharges. The developed numerical model is used to simulate the dynamic hydrological process and and quantitatively represent the three-phase conceptual model from June 2007 to June 2010. Simulated results of two springs' discharges match reasonably well to measurements with correlation coefficients 0.891 and 0.866 at Spring Creeks Springs and Wakulla Springs, respectively. The impacts of sea level rise on regional groundwater flow field and the relationship between inland springs and submarine springs are evaluated as well in this study.

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Effects of Adsorbent Material Properties on the Selective Separation of Non-ideal Multicomponent Fluid Mixtures

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ABSTRACT

A great deal of effort has, thus far, been put into screening thousands of existing microporous materials, including zeolites and metal-organic frameworks (MOFs), for their ability to selectively adsorb desired molecules from a fluid mixture on the basis of molecular size and shape. [1,2] However, difficulties arise when different molecules have similar sizes or lack characteristic structures whose complement can be readily engineered in a microporous material. A lack of fundamental understanding of the structure and thermodynamics of non-ideal mixtures adsorbed on the surface of the material, and the properties of the material itself still precludes the rational design of adsorbents that can selectively separate single components from fluid mixtures.
To this end, we use computationally efficient Monte Carlo (MC) simulation methods [3] to study the adsorption of prototypical coarse-grained multicomponent supercritical fluid mixtures, in porous media. We demonstrate an extensible methodology for studying multicomponent adsorption which yields the complete free energy surface of the confined mixture. This is turn produces a rigorously complete thermodynamic picture of the adsorption process. We focus specifically on non-ideal binary mixtures where previously developed analytical theories, such as Ideal Adsorbed Solution Theory (IAST), struggle to accurately describe the thermodynamics at the adsorbent's interface. [4] This allows us to interrogate fundamental aspects of multicomponent adsorption in porous media for various classes of mixtures when the species have significantly different molecular sizes, interactions with each other and the porous media, and pairwise additivities. We also investigate the specific effects that adsorbent material properties such as flexibility and pore size can have on the selective adsorption of individual components from such classes of mixtures. This allows us to propose general heuristics for the design of adsorbent materials to achieve targeted separation of various classes of fluid mixtures.

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Elastic constants and conductivity of porous materials with isometric or anisometric pores and their prediction via cross-property relations

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ABSTRACT

The porosity dependence of elastic constants as well as thermal and electric conductivity has been a mainstay of materials science for decades. However, only recently it has been shown that a simple cross-property relation [1], derivable from either power-law or exponential relations [2], is able to predict reliably the relative Young's modulus from the relative thermal or electrical conductivity and vice versa. The remarkable feature of our cross-property relation for isotropic porous materials with isometric pores is that it is sufficiently universal to be valid for an enormous variety of different microstructures, ranging from materials with convex pores in periodic or random arrangement (overlapping or not) to periodic or random cellular materials (open Kelvin or random foams and their inverse foam variants, as well as closed Kelvin and random foams) and even materials with concave pores (again in both periodic and random arrangement). In this paper this cross-property relation for isometric pores is recalled and a recently introduced generalized version of this cross-property relation is presented that seems to valid even in the case when the pores degenerate to randomly oriented pore channels or microcracks. Numerical modeling on digital microstructures [3] has been used to validate this new and our classical cross-property relation between the Young's modulus and conductivity [1], and the porosity dependence of other elastic constants (shear modulus, bulk modulus) is discussed as well, including the difficult problem of predicting the effective Poisson ratio of porous materials, on which numerical modeling on digital microstructures has recently shed new light.

Acknowledgment: This work is part of the project "Preparation and characterization of oxide and silicate ceramics with controlled microstructure and modeling of microstructure-property relations" (GA15-18513S), supported by the Czech Science Foundation (GACR).

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Characteristic Fracture Spacing in Primary and Secondary Recovery from Naturally Fractured Reservoirs

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ABSTRACT

We showed previously (Gong and Rossen, 2014a,b) that, if the aperture distribution is broad enough in a naturally fractured reservoir, even one where the fracture network is highly inter-connected, most fractures can be eliminated without significantly affecting the flow through the fracture network. During a waterflood or enhanced-oil-recovery (EOR) process, the production of oil depends on the supply of injected water or EOR agent. This suggests that the characteristic fracture spacing for the dual-porosity/dual-permeability simulation of waterflood or EOR in a naturally fractured reservoir should account not for all fractures but only the relatively small number of fractures carrying almost all the injected water or EOR agent. In contrast, in primary production even a relatively small fracture represents an effective path for oil to flow to a production well. Thus in primary production the effective fracture spacing should include all the fractures. This distinction means that the "shape factor" in dual-permeability reservoir simulators and the repeating unit in homogenization should depend on the process involved: specifically, it should be different for primary and secondary or tertiary recovery. We test this hypothesis in a simple representation of a fractured region with a non-uniform distribution of fracture flow conductivities. We compare oil production, flow patterns in the matrix, and the pattern of oil recovery around fractures with and without the ”unimportant” fractures present. In primary production, all fractures much more permeable than matrix play a significant role in production. The shape factor or repeating-unit size should reflect the entire fracture distribution. In secondary or tertiary production, the role of fractures that carry relatively little flow depends on a dimensionless ratio of characteristic time for matrix and fracture flow, and the ratio of flow carried by the different fractures. In some cases, the appropriate shape factor or repeating-unit size for waterflood or EOR should reflect only those fractures that carry most of the flow.

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Estimating Apparent Thermal Diffusivity Using a Discrete Fourier Transform Bootstrap (DFTB) Method

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ABSTRACT

A discrete Fourier Transform bootstrap (DFTB) method was developed and compared to traditional methodologies for estimating apparent thermal diffusivity. The data sets used to perform this analysis were collected from three different regions: tropical rainforest, desert, and from an undifferentiated highland. It showed to be comparable to traditional methodologies and less sensitive to fluctuating solar irradiation common in many settings, e.g. under-canopy environments. The focus of this work is to provide a more in-depth analysis of the method, showing its capabilities to estimate the apparent thermal diffusivity in dynamic saturation values and at different seasons and periods throughout the year.

In the past, the data collected to analyze the DFTB method were taken at the different sites for a time span of roughly 40 days. A rain-free period was then found from each set. As a result, the data length for each site varied and the soils had near-static saturation values. Here we use 15-day data sets for each month at each site without discriminating the saturation value of the soil, meaning that some of the data sets have a mixture of rain-free and rainy data. The results are then compared with each other for different seasons of the year and between months. At the same time dry and wet data sets, of the same length, are compared to show its validity at varied conditions.

A broad range of data sets were used to analyze the capability of the DFTB method to climatically different environments for different seasons of the year and for varying soil saturation values. These results show the robustness of the DFTB method and its broader applicability. Furthermore, the general agreement of the results allows for:
- Better understanding of the heat transport in the shallow subsurface.
- More accurate heat-transfer models where the apparent thermal diffusivity estimate is of great importance.

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Modeling of water intrusion control in a porous media with the injection of relative permeability modifiers dispersed in gas phase

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ABSTRACT

In some Colombian gas-condensate reservoirs, water intrusion causes the wellbore to stop flowing. This issue is due to active aquifers that produce a continuous movement of the water-oil contact. When the water-oil contact arrives to the near-wellbore zone, the water production increased rapidly, and the invasive water saturates the pores, and it generates blockages to the gas and oil flow. As a consequence, severe reduction in the field production can take place. To avoid this condition, a recent wellbore chemical technique has been developed for improving flow conditions in porous media. It is based on the injection of chemicals dispersed in the gas phase. The chemicals are named “relative permeability modifiers”. The invasive gas push down the water-oil contact and the relative permeability modifiers are dissolved in the water. These chemical agents are absorbed on the mineral surface of the porous media, and it produces a changes on the capillary and interfacial forces between the rock and the water. The modifications on interfacial forces make that the water becomes less mobile, and the water-oil contact reduces their move velocity. Thus, the rock becomes in a system “strongly water wet”. On other hand the technical/economic success or failure of the wellbore intervention depends on physical & chemical phenomena of chemical flooding into the reservoir. Some phenomena include chemical transport, dissolution of chemical agent with the water, and adsorption. Therefore, it is necessary to model and simulate the predominant phenomena in order to quantify the reduction of water production when this technique is used. However the existing predictive models of the relative permeability modifiers injection in a dispersed way not include some relevant process as e.g. the dynamic adsorption. In this work we model the injection of relative permeability modifiers dispersed in gas phase into a porous media. It is represented through multiphase/multicomponent reservoir simulator. The model takes into account this chemical agent transport, mass transfer between the gas and the water, and the dynamic adsorption on rock walls. The chemical transport equation takes into account the advective and diffusive mechanisms via Darcy macroscopic equation and Fick law. The finite-volume method is used to solve the resulting equation system. This model can be used to predict the water production reduction when is injected relative permeability modifiers.

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Reinforcement of RC structure by carbon fibers

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ABSTRACT

In recent years, rehabilitation has been the subject of extensive research due to increased spending on building work and repair of built works. In all cases, it is absolutely essential to carry out methods of reinforcement or repair of structural elements, and that following an inspection analysis and methodology of a correct diagnosis.
This research focuses on the calculation of the necessary reinforcement sections of carbon fiber for structural elements with reinforced concrete in order to improve their load bearing capacity and rigidity. The different results obtained revealed a considerable gain in resistance and deformation capacity of reinforced sections without significant increase in the weight of the rehabilitated elements.

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Haines jump dynamics using multi-phase free energy lattice Boltzmann simulations

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ABSTRACT

Recently, the development of micro-CT imaging equipment has enabled the direct observation of pore scale flow events in porous media flow. This has important implications for applications including CO2 storage and Enhanced Oil Recovery. Recent observations include Haines jumps [1,2], events associated with an abrupt increase in the fluid velocity and a sudden drop in capillary pressure, as the interface jumps from a narrow restriction into a wider pore body with the non-wetting phase (e.g., CO2 or oil) displacing the wetting phase (water). This leads to fluid redistribution in the surrounding area of a draining pore, as a significant fraction of the non-wetting phase, required to drain the pore-body, is supplied by imbibition occurring in the neighboring pore throats.
Here we use multi-phase lattice Boltzmann (LB) simulations to verify the Haines jumps observed in the experiments. For this purpose, we developed a free energy Multiple Relaxation Time (MRT) LB algorithm, including multi-GPU implementation for large computational domains. First, we investigate displacement in simplified three dimensional geometries (micro-fluidic geometries). We verify that these interfacial jumps are associated with both drainage and imbibition dynamics. We recently validated that the method can capture the correct dynamics for imbibition, ensuring that the rate at which non-wetting phase is provided for draining the pore-body is correctly resolved. As the fluid velocity during a Haines jump event can be much larger than the average velocity, correctly capturing the displacement process requires solving the full Navier Stokes equations. Examining the duration of higher interfacial velocities during a Haines jump event reveals that this coincides with the end of fluid rearrangement in the surrounding pore throats. Therefore, this is determined by the amount of non-wetting phase in the neighbouring pore throats and the time-scale over which high transient pressure gradients can be sustained. Second, we consider realistic three dimensional pore space images of real rocks. We observe interfacial jumps into the draining pore, in agreement with experiment. We conclude that the Ohnesorge number (ratio of viscous forces to inertia and surface tension) plays a crucial role in the Haines jump dynamics and the identification of the type of pore filling dynamics that will occur. Finally, we examine the effect of Haines jump events on relative permeability calculations on three dimensional pore space images of real reservoir rock samples.

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Enhancing Mechanical Properties of Polymeric Foams with Functionalized Cellulose Nanocrystals

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ABSTRACT

The aim of this research is to investigate the effect of hydrophobically functionalized cellulose nanocrystals (CNC) on mechanical properties of porous poly(high internal phase emulsions) (poly(HIPEs) structures), a polymer foam. CNCs isolated from tunicates (t-CNC) were subjected to partial silylation with isopropyldimethylchlorosilane (IPDMSiCl) at 2, 4 or 6 equivalents relative to the cellulose repeat anhydroglucopyranose unit (AGU) in toluene. The hydrophobically functionalized t-CNCs were characterized by techniques such as ATR-FTIR, WAXD, TEM and XPS. It was found that degree of substitution of the modified t-CNCs increased with increasing IPDMSi/AGU ratio, while the crytallinity index decreased from 94% to 73%. TEM images t-CNC showed decrease in average thickness of nanocrystals from 16 nm for unmodified t-CNC to 10 nm for highest substituted t-CNC. Poly(HIPE) was synthesized via polymerization of a water in oil HIPE. The oil phase consisted of functionalized t-CNCs added into an acrylate monomer mixture. Hydrophobically functionalized t-CNCs were easily dispersed in the monomers by overnight stirring with a magnetic stir bar. Regardless of substitution degree, incorporation of 1 wt.% t-CNCs in poly(HIPE) led to more than 100% increase in modulus of the wet poly(HIPE)s. Skeletal densities (determined by helium pycnometry) were in the same range for all of the samples. BET surface areas of the nanocomposite samples were higher than the neat sample. SEM micrographs revealed smaller but more uniform voids in the samples containing the modified t-CNCs, suggesting that the impact of the CNCs on properties is more than simple reinforcement.

Design of functionalized alumina monoliths for protein purification

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ABSTRACT

Protein purification has been a long-standing engineering challenge. The more conventional chromatography methods are characterized by limiting diffusional transport of solutes rendering considerably slow protein isolation processes, resulting in low production yields and higher product costs [1, 4]. Monoliths are hierarchal porous structures comprising micro to nanometer sized pores and channels, leading to the improvement of the convective component of solute transport through the chromatography column [2]. In the current work, novel highly porous inorganic monolithic columns were developed using gel casting technique in combination with emulsification [3]. ?-Alumina green bodies were prepared by making an emulsion using a suspension of alumina as the continuous phase and different lipids, such as corn oil, castor oil, margarine and their combinations, as the dispersed phase. The rheological properties of the emulsions showed shear thinning behavior under emulsification conditions and their rheology was related to the fraction of dispersed oil droplets by a simple power law expression. The method has proved to be robust as seen by the high heating rates used for early stages of burnout without fractures or collapse during sintering. Varying pore morphologies and modalities were observed in the final sintered cellular structures (Figure 1) when using additives (lipid and gelling agent) providing different rheologies. Analysis of scanning electron microscopy images and results of mercury intrusion porosimetry (Figure 1, 2a & 2b) showed that the average pore size varied between 1.8 - 15 μm depending on the additives present. The average pore size was found to be inversely proportional to the viscosity of the emulsion. Average porosity was found to be in the range of 25% - 58% (Figure 3). The pores of the obtained monolithic columns were further modified with (3-Aminopropyl) triethoxy silane (APTES) to obtain final amine ligand groups to which the substrate protein will attach. The modification was characterized by SEM-EDS (Figure 4), FTIR and NMR measurements. Further analysis with X-ray micro-tomography will be carried out to map the morphology and apply existing models to understand the entailing flow dynamics in these columns.

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Multiscale Characterization of Spatial Heterogeneity from Optical Photographs of Oil Shale

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ABSTRACT

Oil shale as an unconventional resource contains significant potential for future petroleum and energy supply. The largest reserves are concentrated in the Eocene Green River formation in the United States and are estimated to contain ~4 trillion barrels of oil in-place (Birdwell et al., 2013). Production from this thermally-immature organic-rich rock is primarily through in-situ thermal heating, which leads to the conversion of the solid organic matter (kerogen) into producible oil and gas. It is also known that many of the thermo-mechanical properties of the source rock (e.g., thermal conductivity, Young's modulus), relevant in said in-situ retort operations, are strong (and often sole) functions of their kerogen content (Baughman, 1978); an essential input in field-scale simulations.

Here, we present a workflow through which we have obtained detailed multiscale characterizations of the spatial heterogeneity from optical photographs of oil shale cores. In the first part, we shall discuss a novel experimental technique for quantifying kerogen content from optical photographs, which produces estimates covering scales of a few hundred microns to several hundred feet. It is simple, cheap, non-invasive, and requires no complex instrumentation other than an ordinary camera. Maximum error bounds are ±4wt% TOC (total organic carbon) or ±10GPT (gallons of oil per tonnage of rock). We shall then discuss how the deterministic information obtained from the previous step is used to construct a geostatistical description of the spatial heterogeneity. It is shown that such a description can be useful in supplying missing fine-scale information from routine well-log/lab measurements at other wells.

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PIV measurements within a randomly packed bed of spheres

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ABSTRACT

Particle image velocimetry (PIV) has been used to investigate the dynamics of the flow in a randomly packed bed of mono-sized spherical particles at pore Reynolds number, Rep, between 30 and 4000. The studied bed is transparent and also the refractive index of the liquid is matched with the spheres to provide optical access to the flow within the bed without distortions. The PIV measurements indicate that the flow is no longer in the creeping regime at Rep ? 100 while integrated pressure drop data yields that it is. This shows that detailed measurements can yield more information of the overall flow field than measurements of integrated quantities. Statistical analysis of the spatial distribution of time-averaged velocities shows that the velocity distribution is self-similar with respect to Rep for laminar flow and for turbulent flow. The probability for relatively low and high velocities decreases with Rep while recirculation zones that appear in inertia dominated flows are suppressed by the turbulent flow at higher Rep.

Experimental study of CO2 dissolution – convection phenomenon at high pressure

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ABSTRACT

The density driven convection phenomenon has a significant role in enhancing the CO2 geological storage capacity. Deep saline aquifers are targeted for large scale geological sequestration. Once the CO2 is injected in saline aquifer, the supercritical CO2 rises up, forms a thin layer of free phase CO2, and the dissolution and molecular diffusion of the dissolved CO2 in brine begins. The CO2 saturated brine is denser than the original brine leading to gravitational convection of CO2 saturated brine. Convection accelerates the dissolution process and thus improves the safety and the efficiency of the sequestration.
Laboratory experiments have been previously performed with experimental set-ups allowing the visualization of the phenomenon (1) eventually combined to the measurements of the dissolved CO2 mass transfer (2) as a function of the permeability of the medium. The visualization of the process was possible as Hele-Shaw cells at atmospheric pressure were used. Pressurized cylindrical vessel containing porous media allows measuring mass transfer of CO2 using the pressure decay concept (3) but visualization of the convection/dissolution was not possible for these setups.
In this work, we performed experiments in a pressurized transparent cell similar to a Hele-Shaw cell but with bigger aperture. Permeability was varied by changing the size of the glass beads filling the cell. Bromocrysol green was used as a dye to track the pH change due to the presence of dissolved CO2 (1). The phenomenon is captured by a high resolution camera. We studied the effect of the pressure and of the permeability on the fingering pattern, the onset and the timescale of the phenomenon and the quantitative mass transfer of dissolved CO2. Experiments were validated on numerical simulations performed using STOMP (Subsurface Transport Over Multiple Phases) developed by the PNNL (Pacific Northwest National Laboratory) Hydrology group of the Department of Energy, USA.

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Experimental Study of Propane Condensation in Nano-Fluidic Chips

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ABSTRACT

Prediction of unconventional reservoir production characteristics depends on the understanding of hydrocarbon phase behavior confined in nano-pores. It is well recognized that under nano-confinement, the phase behaviors of fluids are different from those observed in the bulk state. There are, however, few experimental studies that directly visualize the differences in the phase behavior between bulk and that confined in nano-pores (Luo (2015), Parsa (2015), and Wang (2014)).
In this study, we utilized transparent nano-fluidic chips to observe phase transition of a research grade, 99.99% pure propane at room temperature [65 – 70 ?F]. Each chip has three different sets of channels that the smallest channels have nanometer depth. 10 nm chip is the chip that its smallest channels are 10 nm deep. Here we used 10 nm, 30 nm, 50 nm, 300 nm, and 500 nm chips. Propane pressure is varied using a hand operated piston pump. Phase behavior is observed by a microscope which is capable of taking still images or video clips. Pressure is increased by the pump until propane condensed inside the nano-fluidic chip (condensation point). Thereafter, pressure is decreased until the condensation vaporized (vaporization point). At a constant temperature, condensation and vaporization pressures were generally not equal and demonstrated hysteresis.
We compared the observed propane condensation pressures to those predicted by Peng-Robinson (PR) equation of state and those provided by the National Institute of Standard and Technology (NIST). Propane condensation pressure in 500 nm chip is almost identical to those provided by NIST and PR EOS. But propane condensation pressures in 300 nm, 50 nm, 30 nm and 10 nm chips are lower than those given by NIST and PR.
In order to predict and justify our experimental results we combined the Kelvin equation and Local Density Theory (LDT) with PR EOS. Mohammad (2009) and Ma (2014) modified Peng-Robinson equation of state by LDT in order to include the effect of the confined fluid interactions with pore walls in fluid phase behavior. Based on our calculations Kelvin equation lowers the predicted condensation pressure by PR EOS fairly close to our experimental results. But in our experimental pore size range (500 nm – 10 nm) LDT does not add a significant effect of confinement to the condensation pressure. For example in 10 nm chips Kelvin equation decreases the condensation pressure by more than 10 percent while LDT only shrinks it by no more than 0.01 percent. To further improve our modeling a modified Kelvin equation is derived with less assumptions and it lowered the predicted condensation pressure in 10 nm chips by additional 0.3 percent (0.3 psi).
Figure 1. General set up of the propane phase behavior experiments using nano-fluidic chips (not to scale).

Figure 2. 30 nm nano-fluidic chip used for propane phase behavior experiments. Channels marked as 1 and 2 are microchannels. Channels in the network marked as 3 have width of 3 μm and depth of 30 nm.

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Direct visualization of dispersion under two-phase conditions; a micro-model study

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ABSTRACT

Dispersion in porous materials can be found in various applications such as environmental engineering, contaminant hydrogeology, petroleum engineering, soil physics, and food processing industry. Although dispersion in single-phase flow has been intensively studied, the knowledge about dispersion under two-phase conditions is not well established. Using a novel visualization setup, solute transport in a poly-dimethyl-siloxane (PDMS) micro-model under two-phase flow conditions was visualized and monitored for the first time. We were able to visualize and characterize transport under two-phase flow delineating the non-Fickian behaviour induced by phase occupancy. The obtained real-time images illustrate that under two-phase conditions, hydrodynamically stagnant zones are created which do not contribute to the transport by advection. This effect induces the deviation from the Fickian transport. We have been able to visualize the mobile and immobile zones inducing non-Fickian transport under multiphase flow conditions. This study provides sound evidence that the parametrization of transport in a single-phase system cannot be applied to multiphase flow conditions, and phase saturation should be included in the analysis.

Geo-electrical characterisation in the context of geological carbon sequestration

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ABSTRACT

The effects of CO2 emission which contribute to global warming that lead to the effect of climate change can be minimised by carbon sequestration technique. However, it has been argued that there is possibility of CO2 leakages from the storage reservoirs to shallow aquifer and contaminate portable groundwater which consequently become a threat to living organisms. The method for the detection and monitoring of potential CO2 leakage in any storage depth is paramount in the risk assessment framework. Meanwhile, the current monitoring techniques such as time-lapse 3D seismics are very expensive which may not be affordable by low income countries. In order to develop a low cost suitable monitoring strategy for injected CO2 into porous domain such as silica and carbonate sand, simultaneous measurements of electrical conductivity (?b) and dielectric constant (?b) using time domain refractometry (TDR) have been carried out at high pressure and temperature relevant for geological storage of CO2. The effects of pressure, temperature, salt concentration and porous materials on geoelectrical properties (?b, ?b) and water saturation (Sw) relationship have been studied in this work.

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Temperature dependence of elastic properties of porous alumina-mullite composite ceramics – From micromechanical property predictions to indications of a mullite phase transformation

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ABSTRACT

Alumina-mullite composite ceramics are highly refractory materials. The deliberate introduction of porosity into these ceramics reduces the thermal conductivity and heat capacity of these materials, which makes them more suitable for high-temperature thermal insulation and furnace linings in cyclically operated equipment. However, their high-temperature elastic behavior has not been investigated until recently. This work deals with the preparation of porous alumina-mullite composite ceramics by starch consolidation casting with different contents of potato and corn starch (15, 30 and 45 vol.%, related to the solids) and firing at 1570 °C (during which the organic phase burns out). Mullite contents were 10, 20, 30 wt.% (A90M10, A80M20, A70M30; A – alumina, M – mullite) and the porosities attained were in the range 28.6–55.1 %, with pore sizes determined by the starch type (< 50 µm for potato starch, < 20 µm for corn starch). After calculating the Voigt-Reuss-Hill averages for the Young's moduli of the three types of dense composite ceramics, the porosity dependence of the Young's modulus of these materials was predicted on the basis of model relations (power-law and exponential) and compared with experimental values (obtained via the impulse excitation technique from flexural vibrations of bars) […]. The range of measured Young's moduli is 29–144 GPa, being dependent on the composition and porosity of the materials. As expected for porous materials with convex pores, it has been found that the measured data are in good agreement with the exponential predictions, whereas the power-law predictions are much too high. For selected samples the measured temperature dependence of the Young's modulus was compared with predictions based on the temperature dependence master curves for pure alumina and mullite. The composite ceramic with the highest mullite content (A70M30) exhibits a clear anomaly in the temperature range 900–1200 °C that might be further evidence to the structural phase transformation postulated by Hildmann and Schneider [1] and Schreuer et al. [2], see also Schneider et al. [3].

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The Experimental Study of Horizontal Redistribution

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ABSTRACT

Traditionally, multiphase flow in porous media is described by the extended two-phase Darcy's Law, which is based on Darcy's Law by adding the relative permeability. The driving force is only pressure gradient for the horizontal direction, which means flow will cease without pressure gradient. However, this is contradicted by some experimental evidences. Also, there exist theories based on thermodynamic approaches that propose the presence of other driving forces in two-phase flow. In particular, the following generalized Darcy's Law has been proposed:
v_?=-(k_r? K)/?_? [(?p_?-?_? g)+?_? ?a_wn+?_? ?S_?]
where v_? donates ?-phase relative velocity with respect to solid, K donates the intrinsic permeability, k_r?, S_?, ?_?, p_? and ?_? represent the relative permeability, saturation, viscosity, pressure and mass density of ?-phase, respectively, a_wn is the specific fluid-fluid interfacial area, and ?_? and ?_? are material properties. This equation suggests that it is possible to have a pressure gradient even if there is no flow. In that case, ?p_?, ?a_wn and ?S_? could balance each other.
In this work, we investigated the validity of this equation through the study of horizontal redistribution of fluids in soil. Homogeneous sand was packed into a horizontal flume, which was divided into two domains by a thin metal sheet. The initial water saturations were uniform for each domain but they were different for the two domains. By removing the metal sheet, water from wet domain started inflow into the dryer domain. Both water and air pressures and water saturation were measured over time and positions. Gamma rays system and pressure transducers were employed for the saturation and pressure measurements, respectively. The experiment was finished when the equilibrium established and flow ceased. Then, the sand was cored at several positions and the interfacial area was calculated. The data will be used to check whether a pressure gradient existed in the flume under no-flow conditions. Then, material coefficients ?_? and ?_? will be determined, and their dependence on saturation or pressure will also be investigated.

A Computational Model for the Charging Process of a Sorption Heat Storage Device by Radio Waves

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ABSTRACT

In current designs, charging thermochemical heat storage devices proceeds either by providing heat via heat exchangers linked to a separate heat transfer loop (indirect concept) or by bringing an inert, gaseous heat transfer fluid into direct contact with the solid storage material by, e.g., pumping it through a particle bed (direct concept). In both cases, the entire reactor will be heated up causing significant sensible heat losses and placing certain restrictions on the achievable power. Kraus et al. [1] found experimentally that the dielectric permittivity of zeolites strongly depends on the water loading. Since the dielectric heating power depends on the imaginary part of the permittivity, this effect suggests the possibility of selectively heating the storage material and thereby reducing sensible heat losses.

We present a continuum model describing heat and mass transport through zeolite pellet beds, the sorption process and the coupling to an externally supplied radio wave field. The model is implemented into the finite element software OpenGeoSys as a monolithically coupled process. It is used for simulating the dielectrically driven desorption of water from zeolite pellets in a directly permeated fixed bed reactor. We numerically asses the amount of energy savings and heating powers possible in comparison to conventional regeneration methods. Our findings will help to evaluate under which conditions radio waves are a viable option to charge zeolite-based heat stores for applications like Power-to-Heat. The model can further serve as the foundation for other applications, such as catalytic gas decontamination, where dielectric heating enables novel continuous process designs.

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Filling box flows in porous media

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ABSTRACT

Drawing on ideas from turbulent plume theory, we present a novel solution for buoyant convection from an isolated source in porous media of finite extent. As depicted in figure 1, we divide our problem in three flow regimes: (i) a negatively-buoyant plume, (ii) the laterally- or radially- outward motion of discharged plume fluid along the lower (impermeable) boundary in the form of a gravity current, and, (iii) the subsequent ascending motion of this discharged plume fluid towards the source after the gravity current reaches the (impermeable) vertical walls.

By considering the plume to be in a Darcy regime with Pe > O(1) and the flow to be Boussinesq and miscible, we derive a self-similar solution. Our approach is therefore similar to the classical analysis of Wooding (1963) except that we replace his (constant) diffusion coefficient with a velocity-dependent dispersion coefficient, which necessitates a division of the descending plume flow into inner and outer regions. On the basis of this solution technique, we derive new expressions for the variation of the plume volume flux and concentration as a function of the distance from the source, the permeability, the buoyancy flux, etc. (Sahu & Flynn, 2015a,b).
Of course, when the plume encounters the bottom of the control volume, an outflow of dense fluid occurs. The plume outflow condition prescribes the gravity current inflow condition. Using this result along with existing self-similar solutions that describe the motion of a gravity current through porous media, we are able to predict the gravity current height, length and speed as functions of time.

After the gravity current front reaches the vertical sidewalls, discharged plume fluid advects upwards towards the source. The interface between this dense fluid and the overlying ambient fluid is termed the “first front”. We find a solution for the motion of the first front by applying a volume flux balance equation.

By synthesizing the above three flow regimes, we develop a “filling box” model that can predict the time needed for dense source to fill the control volume up to the point of overflow as a function of the source and reservoir parameters.

For purposes of corroborating our model predictions, complimentary laboratory experiments were performed in a rectilinear geometry with fresh water and salt water as the working fluids. Images were recorded during the experiments and later post-processed in matlab by employing an interface detection algorithm to determine the height profiles of the gravity current and the first front. We find good agreement between the measured and predicted height profiles (Sahu & Flynn 2015a).

Extending the above results to a nonuniform porous medium, we also study the effects of sudden permeability changes in a filling box flow. This new investigation is primarily similitude experimental-based and entails varying the ratio of upper and lower layer permeabilities from 1/25 to 25. A sample experimental image with k(upper)/k(lower) = 9 is shown in figure 2. Here, in contrast to

figure 1, not all of the plume fluid reaches the bottom of the control volume. Rather some significant fraction propagates along the (horizontal) interface between the upper and lower layers as an intrusive gravity current exhibiting fingering instabilities along its bottom surface.

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ENHANCING THE BEHAVIOR OF COLLAPSIBLE SOIL USING BIOPOLYMERS

Presenter: Mohamed Ayeldeen
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ABSTRACT

Due to increase of land development all over the world, the need to deal with problematic soils such as collapsible soils became vital. Collapsible soils are widely distributed in most parts of the world. Such soils cause potential construction problems due to their collapse upon wetting as reduction in strength, excessive and sudden settlement when it becomes wet leading to failure of the structure.
This study aims to investigate the mechanical behavior of collapsing soil treated with two types of biopolymer (xanthan gum, and guar gum). Biopolymer is a natural polymer produced by living organisms. Therefore, Biopolymer is considered as environmentally friendly and sustainable material. The program included measuring the collapsing potential, compaction characterizations and shear strength for collapsible soils stabilized with different biopolymer concentrations. The results indicated significant decrease in collapse potential, while maximum dry unit weight and the optimum moisture content are increased. Cohesion stress significantly increased as biopolymer concentration increased for both unsoaked and soaked specimens.

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Effect of iron-bearing minerals on surfactant adsorption

Presenter: Travis Comer
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ABSTRACT

A declining number of oil field discoveries has led to an increased interest in enhanced oil recovery (EOR) technologies to produce residual oil and gas deposits where natural pressure drives and artificial lift capabilities have been exhausted. A technique whereby surfactant solutions are injected into reservoirs to reduce the oil/water interfacial tension, alter the wettability of the reservoir rocks (e.g., carbonates) and maintain a favorable endpoint mobility ratio is now approaching economic viability. Surfactant losses due to adsorption within the reservoir, however, drive up the cost of the application and is one of the major hurdles to be overcome with this EOR technique. The purpose of this research is to examine the effect of iron-bearing minerals within the reservoir on surfactant adsorption rates. To observe these effects, a series of dynamic adsorption measurements will be conducted using sandpacks containing varying amounts of iron-bearing minerals, including siderite and others, using different type of surfactants such as sulfates, carboxylates and sulfonates under various temperatures. These flooding experiments are being performed by using 99% pure silica sand and prepared with a narrow particle size distribution range of 53–75 microns for the sake of repeatability. To ensure homogenous distribution throughout the sandpack, the sand is poured into a polyimide sleeve through a custom-made sieve device that is composed of up to 5 mesh filters attached to a vibrating platform. The sandpack is then solidified using a technique pioneered at UH. The details of this technique will be presented. To measure the rate of adsorption, iron and surfactant concentrations will be monitored in the produced fluids along with changes in oil saturation. Ion concentrations will be measured, and Gas Chromatographic (GC) and High Performance Liquid Chromatographic (HPLC) analyses will be employed to measure the effluent composition. With this new understanding, surfactant formulations can be made in order to counter the potential surfactant losses within the reservoir.

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Modeling of Transport Phenomenon in Arthroscopic Laser Surgery

Presenter: Pradyumna Ghosh
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ABSTRACT

It would provide tremendous benefit by addressing quality and safety issues such as laser intensity and time for exposure to achieve the required therapeutic effects. However to achieve the above requires working on a number of fundamental physics simultaneously since the media involves heat and mass transfer simultaneously in biological tissues. The thermal effect depends on the tissue, its composition and water content as well as the age of the patient. Simplifications are imposed in modeling the laser heating considering that as a parabolic heating at the boundaries of the biological tissue. Initially a bio-transport mechanism model with phase change has been developed in COMSOL multi-physics for a chicken patty frying where previously published numerical and experimental data were available. Using this validated bio-transport mechanism model for chicken patty a new model involving human tissue which is assumed to be porous in which the different solid matrix properties and fluid properties are defined to take into account the multi-phase change occurring during the application of heat flux in laser surgery, study the transient heat transfer through integral analysis has been performed in COMSOL multi-physics. Last but not the least an effort has been made to understand the transport phenomenon during the arthroscopic laser surgery.

D as in Darcy, D as in diapers: how porous media experts can make the difference in industry

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ABSTRACT

Hygiene absorbent product as well as other consumer goods such as towels and batteries are strongly relying on Porous Media to fulfill their function.
Despite their perceived simplicity, product development requires a good knowledge of the physics involved. This offers career opportunities for young Porous media scientists as well as collaboration with established research groups.
This speech provides a glimpse on how people from the Porous Media academic world can contribute in P&G and ultimately how they can help in improving the life of billions of consumers worldwide.

Structure Generation and Nonlinear Deformation Simulation of Thin Nonwoven Structures at the Micro-Scale

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ABSTRACT

In the presentation at hand the mechanical simulation of compression-recovery tests of thin nonwoven structures is addressed. To this end the generation of virtual nonwovens is regarded. In order to obtain a homogeneous fiber distribution of non-touching fibers with a high solid volume fraction, in a first step a structure with a bigger height and a lower solid volume fraction is generated with the software tool GeoDict, see [1]. In a second step these fibers are coated virtually to ensure an isolation distance between the fibers in the final structure. Then these structures are compressed to obtain the desired high solid volume fraction with the solver FeelMath [2], which is developed at ITWM. This procedure for the structure generation is depicted in Figure 1.

In the second part of the talk the mechanical simulation of compression-recovery tests of the thin nonwovens are addressed. In case of chemically bonded structure as shown in Figure 1 the influence of elastic and viscoelastic binder properties onto the overall behavior of the nonwovens in case of elastic fibers is considered. Furthermore, these studies are extended towards viscoelastic fibers. In a last step the influence of the bond type (e.g. thermo-bonds) onto the compression-recovery behavior is investigated numerically.

Figure 1: Proecdure to generate virtual chemically bonded nonwoven with high solid volume fractions: on the left hand-side the base material is depicted, which is then compressed analogeously as in the production process, on the right-hand side a representative cut-outof the final structure is displayed at the real height of the regarded sheets

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Impact of radiation transfer modeling on the simulation of the thermal response of ablating spacecraft thermal protection systems

Presenter: Vincent Leroy
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ABSTRACT

Many space flight missions imply having a spacecraft enter atmosphere at a certain point. Whatever the atmosphere considered, the entry velocity is such that the spacecraft is submitted to extreme heat fluxes (several MW/m²). The protection of the payload therefore requires the design of a thermal protection system (TPS), made of a material suited for the mission considered. Among these materials are a family of porous lightweight ablators, which convert the heat flux to chemical energy thanks to an endothermic pyrolysis reaction.

Modeling ablation is a challenging task: it involves many physical processes (momentum, heat and mass transfer, chemical reaction, radiation transfer), many of which are highly nonlinear; it also involves high-intensity gradients due to the very high heat flux. Consequently, the modeling of such phenomena is still a open research field, and current models rely as much on upscaling as on heuristic approaches.

In many applications, the temperature at the ablation interface reaches 2000 K and higher, so radiation transfer is assumed to take a significant role in the regions closest to the flow. Most models for ablation, however, do not explicitly model radiation in the porous medium [1,2]. Instead, they include a radiative contribution in the effective conductivity of the medium, implicitly assuming that the radiative conductivity approximation is valid in the entire medium. However, recent developments based on statistical homogenization of radiation transfer defined a validity criterion for the radiative conductivity model [3], and estimates point to questioning the radiative conductivity approximation in the charred layer of the ablating shield, where the gradients are the most intense. However, using a different radiation model would have important consequences on the characterization strategy of materials. Therefore, it is necessary to determine the appropriate model by assessing the sensitivity of the ablation model to the radiation model over a series of well-chosen test cases. The design of the test case suite requires the definition of a reference medium, based on the TACOT virtual material.

For the practical numerical simulation, we couple the ablation simulation code PATO [4] to a Monte Carlo solver for the generalized radiation transfer equation (GRTE) [5]. This choice allows good flexibility of the model, making possible to treat a wide variety of cases and compare them with the radiative conductivity model.

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A Mathematical Model of Fluid Exchange in the Peritoneal Cavity

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ABSTRACT

The peritoneal cavity is a potential space, lined by a thin membrane, which lies within the abdominal cavity. It provides a barrier between the abdominal viscera and the abdominal wall. Under normal physiological conditions, the peritoneal cavity contains very little fluid. Abnormal accumulation of large volumes of fluid in the cavity is known as ascites and is commonly associated with liver diseases. In patients with ascites, a fluid increase of up to 10L can be observed [1], leading to increased hydrostatic pressure and expansion of the cavity. During that time, their physical appearance, mobility and nutrition are affected, as well an increased risk of acute bacterial infection. In severe cases, external dialysis is required to reduce the volume of fluid.

There are several tissues surrounding the peritoneal cavity including the abdominal wall, diaphragm, liver, spleen, and hollow viscera. The aim of this study is to investigate the role played by the surrounding organs in regulating the fluid volume in the peritoneal cavity and the vascular changes in the liver that lead to the formation of ascites.

We developed a compartmental model of the peritoneal cavity with the surrounding tissues acting as sources and drains of fluid. The surrounding tissues are modeled as porous media with varying degrees of hydraulic permeability [2,3]. Darcy's law is used to estimate the rates of fluid flux across the tissue membrane as the volume and pressure in the cavity increase. The model is used to estimate fluid flux contributions of the surrounding tissues under normal physiological states and in extreme conditions, such as those observed in the case of ascites. It is our hope that our research will give us some insight into the formation of ascites, so as to predict the severity of the condition and inform and improve treatment strategies.

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Functionalization of alumina monolithic chromatography columns by self-assembly of (3- aminopropyl)triethoxy silane (APTES): Study of effects of physical parameters and their optimization

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ABSTRACT

Purification of proteins using affinity chromatography is a very common technique. However, it suffers from several problems like diffusion effects and non-specific binding by by-products to active sites. Monolithic chromatography columns provide micro-channels for fluid to flow with minimal diffusion constraints. Effective and homogeneous functionalization, to have highly specific binding sites for molecules of interest, especially inside the pores and channels throughout the monolithic columns, is quite challenging. Silane modification of materials is a common practice to obtain custom ligand groups for various applications. Thin films of (3- aminopropyl)triethoxy silane (APTES) are used to promote adhesion between inorganic substrates and organic groups with a wide range of applications from microfluidics devices to bio-composite materials [1]. In the present work, inorganic alumina monolithic columns, prepared by gel casting, were silanized for chromatographic applications by using a sol-gel method using APTES. The method is adapted from the previous work by Yamaguchi et al [2], wherein, a reaction mixture is constituted in ethanol consisting of a silane precursor (TEOS/APTES), a catalyst (hydrochloric acid) and surfactant (CTAB) and activated by incubation at 60?C. The porous alumina monoliths are then added to this mixture and vacuum is applied to perfuse the pores with the reaction mixture ensuring uniformity of the silanization. FTIR and NMR spectral analysis (Figure 1 a. & b.) of the samples prepared using this modified technique show good covalent attachment of silane groups to the porous alumina monolith and availability of free amine groups for subsequent attachment of other moieties like proteins. The SEM-EDS maps (Figure 2) show good distribution of silanol and amine groups throughout the pore walls. Further, we have evaluated the type of catalyst used [4] and found that by using a base (sodium hydroxide) we obtained more homogeneous distribution of silane groups (Figure 3) with high availability for subsequent reaction as when compared to using acidic catalyst (hydrochloric acid). The presence of surfactant, in this modified method (Figure 3) could lead to non-specific binding of proteins, hence it was eliminated in further experiments. In subsequent studies, it was found that the attachment of silane-amine groups seemed to be adversely affected by increase in relative humidity in the reaction environment. However, when making multiple coatings of silane groups a humid environment seemed to favor better attachment and distribution of the silane groups. Increasing the concentration of precursor seemed to have negligible effect on the process. In the next stages, the performance of these functionalized alumina monoliths will be evaluated for isolation of proteins.

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Adaptation of Escherichia coli to Ciprofloxacin in a microfluidic pore network: The Emergence of Resistance along a concentration gradient

Presenter: Jinzi Deng
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ABSTRACT

Microorganisms in nature have evolved in response to a variety of environmental stresses, which include temperature, pH, substrate availability and aqueous chemistry. As a result, the highest abundance of bacteria is often found in the most optimal microenvironment. When a stressor gradient is introduced, bacteria will preferentially grow at the most optimal location along this gradient, which can change over time with adaptation. Next-generation microfluidic devices now permit previously unattainable levels of control and reproducibility of these dynamic chemical environmental stresses. They also provide a consistently reliable real-time means to quantitatively track microbe abundance along a stress gradient. This approach links the dynamic spatial distribution of model microbes such as Escherichia coli with the micro-scale environment. In this study, a novel microfluidic device with porous media and a selectively photo-patterned in-plane gel barrier were used for in vitro real-time tracking of E. coli abundance in response to gradients in both the antibiotic Ciprofloxacin and selected nutrient substrates across a porous media. Ciprofloxacin and nutrients were injected on one side of the porous media, and mineral media without a carbon source was injected on the other. Hydrogel barriers were selectively photo-polymerized between inlet channels and the porous media, such that the nutrient and antibiotic solutes could diffuse from side channels into the porous media while preventing E. coli escaping from the porous media to the side channels. Preliminary observations suggest that the number of E. coli cells increased over time in regions with lower ciprofloxacin concentration. In regions with higher antibiotic concentrations, cell number initially decreased and then fluctuated, possibly due to oxygen and/or nutrient limitation. The overall distribution of E. coli biomass in the porous media showed good correlation with the linear gradient of stress and nutrients at steady state. The area with the most abundant bacteria is the most optimal environment in the system. Modeling of the mass transport of Ciprofloxacin and nutrients across the porous media has identified the optimal “comfort zone” of enhanced E. coli survival and adaptation. Future work will evaluate E. coli response to other environmental stresses, including nutrient limitation and temperature change.

Thermal characterization of granular porous media in the micro-scale domain

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ABSTRACT

Macroscopic properties of porous materials can be described by their micro-structures [1]. Using this presumption, many studies have been conducted in the realm of pore scale modeling method to estimate macroscopic properties (e.g. porosity, permeability, and electrical resistivity) of porous media by modeling micro-structures (e.g. real shapes of grains, pores, and throats) [2, 3]. In spite of rich literature about the application of the method to study flow and electrical conductivity in porous media, comparatively fewer studies have been conducted to investigate thermal conduction properties such as grain size, and roughness and grain shape effects using this method [4]. By considering thermal contact resistance that has been obtained by modeling roughness, we demonstrate the robustness of the method for predicting the effective thermal conductivity that exhibit a good correlation with experimental data (Fig. 1). According to our results, the modeling of roughness is pivotal to grant reliable estimates of effective thermal conductivity. In addition, we show that by increasing roughness that consequently results in a higher thermal contact resistance the effective thermal conductivity decreases (Fig. 2). However, the decrement is the function of the ratio of effective thermal conductivity of solid to fluid parts in a porous medium. Once this ratio increases, the effective thermal conductivity significantly decreases. We demonstrate that the effective thermal conductivity has a correlation with grain size that is explained by thermal contact resistance.

Furthermore, we investigate the effect of grain shape in thermal conduction anisotropy using pore scale domain. Based on our results, when the temperature field is not parallel to either major or minor axes of grains, the overall heat flux vector makes an angle “deviation angle” with the temperature field. Deviation angle increases by augmenting the ratio of thermal conductivities of solid to fluid and the aspect ratios of grains. Additionally, we show that porosity and surface roughness can considerably change the anisotropic properties of a porous medium whose grains are elliptical shape (Fig. 3).

Fig. 1. The effective thermal conductivity of a reconstructed porous medium as a function of roughness with respect to different solid-fluid conductivity ratios.

Fig. 2. The pore scale modeling estimates of effective thermal conductivities of the reconstructed Utah oil sand sample (the solid points) after applying roughness to grains. Empty circles triangles represent experimental data [5] and triangles are estimated values using weighed geometric mean. A good correlation between the pore scale modeling results and experimental data are noticeable [6].

Fig. 3. Anisotropy ratio as a function of aspect ratio, k_s/k_f, porosity and roughness.

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On the Validation of a Compositional Model for the Simulation of $\co$ Injection Into Saline Aquifers

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ABSTRACT

In this work we apply a recently proposed Bayesian Markov chain Monte Carlo (MCMC) framework [1] to quantify uncertainty in the three-dimensional (3D) permeability field of a rock core. This process establishes the credibility of a compositional two-phase flow model to describe the displacement of brine by CO2 and CO2 storage in saline aquifers. 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.

We employ forward models consisting of a system of discretized partial differential equations along with relative permeability curves obtained by a curve fitting of experimental measurements. We consider a forward model to be validated when: (i) numerical simulations reveal that the Bayesian framework has accurately characterized the core's permeability and (ii) Monte Carlo predictions show excellent agreement between measured and simulated data. A large set of numerical studies with an accurate compositional simulator shows that forward models have been successfully validated. For such models our numerical results show that we are able to capture all the dominant features and general trends of the CO2 saturation fields observed in the core.

Our study is consistent with the design and findings of real experiments.

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Analysis on Stability and Influencing Factors for landslide based on super thickness soil

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ABSTRACT

The research on the factors affecting the landslide formation and the stability of the landslide has been one of the hot spots of scholars in the world in the landslide disaster studying field. The formation of the landslide has a direct relationship with many factors such as geological structure, rainfall, groundwater, earthquake and so on. All the factors are important influence to induce landslide. The real project of super thickness soil landslide has been selected as an engineering background in this paper. The detailed geological topography survey has been introduced in this paper. And the factors affecting stability for this landslide has been described. The geotechnical analysis software FLAC3D has been used to simulate stability for this landslide. The impact on the safety factor of super thick landslide on sliding soil such as friction angle and cohesion are considered. The sensitivity of sliding zone's cohesion ?angel of internal friction and gravity of sliding mass for landslide's stability. The results show that the influence of internal friction angle on the stability of landslide is more remarkable. It's sensitive degree is nearly 7 times of cohesion. The research result also shows that that numerical analysis for established landslide model is reliable. Landslide belongs lapsed sliding, potential location of landslide shear failure occurs in the middle and back-end. The safety factor will increase with the addition of friction angle and cohesion, safety factor will increase when friction angle adds, and the impact of the latter for the slope stability is greater than the former.

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The application of pile foundation reinforcement and inclination correction of high-rise building in the unsaturated soil ground

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ABSTRACT

As the particularity of strong concealment of the pile foundation engineering, some kinds of defect types are often happened, like its insufficient bearing capacity, excessive settlement and uneven settlement. Then, according to the characteristics of unsaturated porous media, puts forward a kind of pile foundation reinforcement and inclination correction technology suitable for high-rise building, especially for the pile have not reached to the bearing layer, the actual is friction pile. Specific application methods are: (a) supplemented raft foundation within the whole foundation, and set aside holes of static pressure pile; (b) implement the static pressure pile, and seal it with cast-in-place concrete for where settlement is large relative to other place, when the supplemented raft foundation strength is reached to 80%; (c) with the reinforcement of the static pressure piles, settlement rate of the original larger side is decreased gradually, and tends to be stable, however, the other side should be continued to keep settlement; (d) with the help of building deadweight, achieved the aims of inclination correction, and also with the compression of raft foundation to the foundation soil, the bearing capacity of friction pile and foundation soil are increased gradually, the subsidence rate of original smaller settlement side is decreased?(e) all the static pressure piles should be sealed and tied down with the raft foundation, except piles have sealed in the (b), when the inclination of the high-rise building meet with the requirements of the standards, and the settlement of the whole foundation become stable eventually; (f) information construction is also necessary to ensure safe and effective. With the compressive deformation to the unsaturated foundation soil, the bearing capacity of friction piles improved obviously, and the bearing capacity of the overall foundation meet the requirements, and eventually in a normal operation. This kind of reinforcement and inclination correction technology's merits are short construction period, safe and reliable, economic and reasonable, convenient construction and easy controlling, and is beneficial to further optimize and improve research of reinforcement and inclination correction.

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A study of imbibition phenomenon in homogenous porous media during oil recovery process

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ABSTRACT

The approximate solution of imbibition phenomenon governed by non-linear partial differential equation is discuss in the present paper. Primary oil recovery process due to natural soil pressure, but in the secondary oil recovery process water flooding plays an important role. When water is injected in the injection well for recovering the reaming oil after primary oil recovery process, it comes to contact with the native oil and at that time the imbibition phenomenon occurs due to different viscosity. For the mathematical modelling, we consider the homogeneous porous medium and optimal homotopy analysis method has been used to solve the partial differential equation governed by it. The graphical representation of the solution is given by MATHEMATICA and physically interpreted.

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Quantitative analysis on double strength reduction method

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ABSTRACT

Double strength reduction method adopts this reduction way, where it utilizes the different reduction coefficients of strength on the cohesion and internal friction angle, which is more rational. However, the research on double strength reduction method still lacks of quantitative analysis and reasonable explanation. In the coordinate system of strength parameters, use definition of FOS, path of reduction, and critical state to analyze the difference between SRM and DRM. These two methods have unity in path of reduction, DRM can be regarded as the SRM where it begins at an "initial virtual strength point" to reduce. The gradual process of slope destruction is the attenuation of strength parameters. In this process, c and tan? follow direct proportion function; At same time, in the coordinate system of strength parameters, the concept of strength reserve can reflected as the gradual process which is "initial strength area" approaches to "critical strength area"; Research of strength reduction method should concentrate on "strength", and the reduction of strength parameters just is a way to achieve purpose of strength attenuation. Definition of FOS and regression analysis all indicate that critical state is intrinsic property of slope, given geometric model of slope, the critical state is a constant, which is not related to initial strength parameters, c' and tan?' conform to inverse function relation.

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A Linear Composite Pressure-Transient Model for Horizontal Wells in Fractured-Vuggy Carbonate reservoirs

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ABSTRACT

Carbonate reservoirs play a very important role in the world's gas and oil resources. Because carbonate reservoir is usually with strong anisotropy, a horizontal or multilateral well drilled in it may extend through a compartmentalized reservoir which consists of layers, sections, or pockets of reservoir with different properties. The reservoir subsections may be commingled or in partial or full communication. Conventional pressure-transient models assume that the entire length of horizontal or multilateral well remains in the same formation with uniform properties. It's necessary for us to build up new models to satisfy the need of well test. In this paper, different kinds of multi-zone reservoir models are established. The models divide the reservoir into blocks that represent the subsections of the reservoir characterized by uniform average properties. An analytical pressure-transient solution is developed for each block with the Neumann condition at the outer block boundaries together with the inner boundary condition appropriate for the particular well type and production condition. The analytical solution is discretized at the inner and outer block boundaries and coupled by the solution for the adjacent blocks by using the continuity of pressure and flux. Adding the production constraint for well creates a matrix problem to be solved for the wellbore pressure together with the pressures and fluxes at the block boundaries. Knowing the flux and pressure conditions at the block boundaries, pressure distributions within the blocks can also be obtained from the analytical solutions. Then pressure transient response type curves are plotted by computer programming and pressure influence factors are also analyzed, playing a guiding role in analyzing pressure response of the multiple wells of different geometry.

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Impact of suspended elements on the drying rate of porous medium

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ABSTRACT

It is well known that simple liquids evaporate from porous media at a constant rate over a rather long period due capillary “re-equilibration” allowing a renewal of liquid around the free surface of the sample, then a decreasing rate is observed due to the development of a dry region from the surface. 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 the presence of elements in the liquid tends to decrease the drying rate (as long as these elements do not go out of the sample). With dilute suspensions, solid or soft colloidal particles are transported and accumulate below the free surface. This region of accumulation behaves as a dry region, i.e. all occurs as if the new top liquid-air interface was just below it, which induces a decrease of the drying rate. Finally the drying rate can be exactly predicted by assuming that the liquid evaporates from below this zone and diffuses up the sample free surface. The situation is more complex with initially concentrated suspensions. Actually recent MRI data with nanoporous materials suggest that, although they behave as dry regions in terms of macroscopic drying rate, these regions are in fact not dry.

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Drying of mixed wet porous media

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ABSTRACT

Drying of 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 medium depends on not only the microstructures of the porous medium but also its wettability. Some porous materials, e.g., GDLs, show mixed wettability, i.e., hydrophilic and hydrophobic pores coexist in porous media. Nevertheless, drying characteristics in mixed wet porous media is still unclear. To address this issue in the present study, pore network modeling approach is employed. In this method, the void space of a porous medium is conceptualized as a network composed of cubic pores connected by cylindrical throats (the throats and pores are also called the ducts). The mixed wettability of the network is characterized by a parameter called the hydrophilic fraction, defined as the ratio of the number of hydrophilic ducts to the total number of ducts in the network. The capillary valve effect due to the sudden geometrical expansion at the throat-pore interfaces are also considered in our model. Owing to the capillary valve effect, there are two types of pore invasion. The first is bursting invasion into a pore from a throat. The other is merging invasion into a pore from two throats. The threshold pressures for these two pore invasion are theoretically derived. The influences of the hydrophilic fraction on the drying processes are explored. In the cases where bursting invasion dominates over merging invasion, the effect of the hydrophilic fraction on drying depends on the contact angles of the hydrophilic and hydrophobic ducts. When pore invasion is dominated by merging invasion, the influence of hydrophilic fraction on drying is not significant.

Drying of Tissue Paper

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ABSTRACT

Tissue production is among the most energy and capital intensive industries in the US. More than 2000 kWh of total energy are needed to produce a ton of tissue paper, with the majority of the energy going toward the drying of the sheet. Drying is also typically the rate limiting step in the manufacturing process, so any increase in heat transfer rate could allow tissue machines to run faster and more efficiently. An understanding of the physics of the drying of the porous tissue sheet is needed to increase both the energy efficiency and the speed of drying.
In this paper we will give an overview of the steps that transform a dilute slurry of swollen wood pulp fibers into a dry tissue sheet in less than one second. We will focus on the Through Air Drying process used in many modern tissue machines, and show how non-uniform air flow through the sheet leads to significantly reduced heat transfer rates in the later stages of drying [1, 2]. We will also discuss the changes in the porosity and permeability that accompany the drying of the tissue web which contribute to the non-uniform airflow.

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Pore Network Modeling of Salt Precipitation in Porous Media

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ABSTRACT

Salt crystallization in porous media or at their surface is a phenomenon of interest in relation with several important applications, such as soil physics, underground storage of CO2, civil engineering and the protection of cultural heritage, to name but a few. Therefore, there is an increasing importance to understanding the processes behind salinization. The phenomenon causes several changes in the physical properties of porous media, and influences the flow and transport of the components of a mixture within the system. Given the negative impact that salt deposition has on various types of porous media, this research aims to study the process of drying-salinization in porous media and its impact on the static and dynamic properties of porous media. But, even though salinization is highly important to a wide variety of problems, it is still not well understood even at the laboratory scale, and in fact it still lacks a comprehensive and detailed model at this scale.
Thus, one goal of this study is to develop such understanding at the laboratory scale. For this purpose we have developed a pore-network simulator to model salt deposition in porous media during transport of brine. Pore network modeling is the standard method of studying flow and transport processes at laboratory scale. The transport mechanisms that are being studied in drying porous media are vapor diffusion in multicomponent systems, capillary flow in the liquid phase, flow in liquid films, menisci moving in the throats and evaporation at the menisci. At the same time, evaporation of saline water leaves the salt crystals on the throats' wall, leading to reduction of the permeability and porosity and, hence, the fluid velocity field. In our approach, we include all the aforementioned phenomena in the simulation.

Non-trivial wettability effects on evaporation from saline porous media

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ABSTRACT

Drying of saline porous media is important in various environmental and engineering applications including CO2 sequestration in saline aquifers, durability of building materials, vegetation, and soil salinity. This process is influenced by the complex interaction among atmospheric conditions, transport properties of porous media and properties of the evaporating solution (Norouzi Rad et al., 2012; 2015; Shokri, 2014). We investigated effects of partial wettability conditions on the evaporation process from saline porous media. Slight changes in wettability may significantly modify the flow and transport processes in porous media which motivated us to investigate the partial wettability effects on the drying of saline porous media with the associated salt precipitation dynamics. To do so, we conducted a comprehensive series of experiments with sand mixtures containing different fractions of hydrophobic grains saturated with NaCl solutions. The sand columns were placed on digital balances to record the evaporative mass losses. Also, an automatic imaging system was set-up to capture dynamics of salt precipitation at the surface and the receding drying front (the interface between saturated and partially wet zone) during the process. The experiments were conducted in an environmental chamber where the relative humidity and ambient temperature were kept constant.

Our results show that partial wettability condition had minor impact on the evaporative mass losses from saline sand packs and the presence of salt reduced the dependency of the cumulative mass loss on the fraction of hydrophobic grains. This is not a trivial result as one may expect reduced mass losses from drying porous media due to the suppression of upward capillary flow as the fraction of hydrophobic grains increases (Shokri et al., 2009). However, this was not observed in our study. Through macro- and micro-scale investigations of the precipitation patterns at the surface, we found that in the case of partially wettable porous media, patchy efflorescence occurs on discrete areas at the surface that grows laterally while in the case of completely hydrophilic sand, crusty efflorescence occurs supressing the evaporation process. In other words, the hydrophobic grains on the surface prohibit precipitation in those areas, leaving parts of the surface open during the evaporation process. This will contribute to further drying of partially wettable porous media as the diffusion resistance through the hydrophobic grains on the surface is less than that of a salt crust formed at the surface of hydrophilic porous media. Also the outer surface of patchy salt structures enhances the evaporation surface. Our results highlight the importance of the preferential evaporation at the surface due to the presence of grains with different wettability which significantly influences the general dynamics of the process in terms of drying rate, precipitation patterns and the dynamics and morphology of the receding drying front delineated by analysing the recorded images. Our findings offer new insights into the evaporation process from partially wettable porous media saturated with saline water and show that salinity not only adversely affects the soil stability, vegetation and crop production but also may increase the evaporative mass losses in mixed wettability systems.

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Drying of suspensions containing micro- and nano-particles

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ABSTRACT

Understanding the fundamental aspects of drying of suspensions is an essential step toward accurate production of particulate matters which is of great importance to a variety of processes such as production of catalysts, powders and pharmaceuticals products. Many of these products are typically produced in spray drying whereby spray generation followed by solvent evaporation leads to the formation of particles with different characteristics. The surface properties and morphology of solid particles emerging from drying of suspensions are strongly influenced by the general dynamics of the drying process as well as the properties of the suspensions. Single droplet drying has become a very useful approach for studying the drying of suspensions avoiding many of the complexity faced on a pilot scale.

In this work, a comprehensive series of experiments is conducted to investigate the drying behaviour of micro and nano silica-water suspensions. To do so, an Acoustic Levitator with a standard operating frequency of 58 kHz was used to study the drying kinetics of a single droplet. Micro and nano-suspensions were prepared with particle sizes of 1-5 microns and 10-20 nm respectively and the effects of varying initial particle concentrations and initial droplet volume on the drying kinetics were investigated. The temporal evolution of the actual droplet was recorded using a high resolution CCD camera. This information was used to calculate the evaporation rate as a function of the size and concentration of the suspended particles. The final solid particles formed at the end of the drying process were subjected to SEM imaging to investigate the surface properties and morphology of the particles. Using the obtained SEM images combined with the measured evaporation curves, we could accurately delineate how the surface properties of final products are influenced by the presence of micro- and nano-particles and their corresponding concentrations. Comparing the morphology of the particles resulted from the drying of micro- and nano-suspensions enabled us to demonstrate the remarkable dependency of the morphology of the final particles on the size of the suspended particles in the evaporating liquid. Our results extend the fundamental understanding of the mechanisms controlling drying of suspensions.

Roof cooling by direct evaporation from a porous roof layer

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ABSTRACT

Growing energy consumption poses a significant threat to the environment. With the new climate agreement, the world has committed itself to unitedly combat climate change and the need to lower energy consumption has become a necessity. Utilising the energy associated to chemical and physical processes may reduce the need of energy consumption for cooling and heating practices in buildings. This concept motivated many researchers to find innovative methods such as solar roofs, green roofs, and evaporative coolers [1-3]. In this work, we investigated the potential of a drying porous layer to moderate roof surface temperature and the heat flux. To do so, customised rectangular Plexiglas columns were packed with three types of sand with well-defined particle size distribution saturated with water with all boundaries closed except the top, which was exposed to air for evaporation. The containers were placed on digital balances to record the evaporation rates. The container packed with sand grains was equipped with thermocouples specifically designed to measure soil temperature. In addition, a thermal camera with a thermal sensitivity of less than 30 mK and a resolution of 640×480 pixels was fixed above the packed sand to record the dynamics of temperature evolution at the surface. A square heat flux sensor (35.1 mm by 35.1 mm) with a thickness of 2.8 mm connected to a datalogger was placed in the middle of the sand pack to measure the heat flux during the evaporation process. The obtained results revealed the great potential of drying porous media to reduce the heat flux through roof via utilising a part of the energy for liquid vaporisation. As particle size decreased the temperature of roof remained lower than the bare roof for a longer time as a result of the presence of more liquid pathways connecting the receding drying front to the evaporation surface, which kept the surface wet for a longer time. Our results present new insights about the physical mechanisms controlling the performance of drying porous media to regulate roof surface temperature.

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