

# InterPore2021

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## Book of Abstracts



# Contents

3D Magnetic Resonance Imaging Studies of Porous Media: From Operando Catalysis to Fluid Transport in Rock Cores 814 . . . . .	1
3D adaptive modelling of transient multiphase flow experiments using the MOOSE framework 84 . . . . .	1
3D-1D coupling on non-conforming meshes via an optimization based three-field domain decomposition approach 628 . . . . .	2
4D Investigation of groundwater remediation using nanotechnology- a synchrotron-based X-ray micro-tomography study 491 . . . . .	3
4D $\mu$ CT reconstruction with improved time resolution for imaging fluid flow in porous media 486 . . . . .	4
A (dual) network model for heat transfer in porous media 642 . . . . .	5
A 6M Digital Twin for Reservoirs 381 . . . . .	5
A DFT study on the effect of strain on the adsorption of gas in tight gas carbonates 382 . . . . .	6
A Darcy scale coupled fluid-thermal framework to model radionuclide transport from a deep disposal borehole 232 . . . . .	7
A Dynamic Hybrid Multiscale Model for Simulating Flow and Mixing-Controlled Reactions in Porous Media 619 . . . . .	8
A Flow Discretization for Conforming Discrete Fracture Matrix Models with Upscaling of Microscale Fractures 687 . . . . .	9
A Graphical Representation of Membrane Filtration with Adsorption 363 . . . . .	10
A Laboratory Study of Foam Coarsening in Model Fractures 61 . . . . .	11
A Maximum Principle Preserving Finite Element Method with Mass Conservation Property for Solving Two-Phase Flow in Heterogeneous Porous Media 738 . . . . .	12
A Novel Technique of Image Analysis on Foam in Fractures 655 . . . . .	13
A Phase-Filed-Based Formulation for Chemically-Assisted Fracture 757 . . . . .	14
A Semi-Analytical Solution for Modeling of Early-Time and Late-Time Countercurrent Spontaneous Imbibition in Porous Media 696 . . . . .	14

A Stochastic Particle-Based Framework for Multiphase Flows in Fractured Porous Media 266 . . . . .	15
A Three-Scale Model for Flow in Paleo-Karst Reservoirs 41 . . . . .	16
A Unified Gas–Alkane Binary Interfacial Tension Calculation for A Broad Range of Pressure and Temperature: A Machine Learning Approach 223 . . . . .	17
A Unified Plot for Fluid Phase Transitions 189 . . . . .	18
A Virtual Element Discretization of a 3D Elastoplastic Problem 515 . . . . .	19
A chronopotentiometric study of polymeric ion-exchange membranes in alcohol-water me- dia 550 . . . . .	19
A detailed pore scale modelling of colloid transport in porous media using lattice Boltzmann method 530 . . . . .	20
A digital workflow for analysis of flow in porous media: Multiphase transport phenomena from pore to field scale in subsurface flow 790 . . . . .	21
A discrete element model (DEM) for swelling behavior of clay 672 . . . . .	22
A dynamic pore network model for imbibition simulation considering corner flow 303 . . . . .	22
A framework to map pore volume change and mineral dissolution/precipitation of wellbore cement exposed to high concentration CO <sub>2</sub> using micro-CT images 426 . . . . .	23
A fully parallel Pore Network Simulator for plug size pore scale simulations 166 . . . . .	24
A homogenised model for flow, transport and adsorption in a heterogeneous porous medium 666 . . . . .	25
A hybrid-dimensional compositional two-phase flow model in fractured porous media with phase transitions and Fickian diffusion 490 . . . . .	25
A level set approach to Ostwald ripening of real gases in porous media 66 . . . . .	26
A macroscopic two-length-scale model for natural convection in porous media driven by a species-concentration gradient 287 . . . . .	27
A midsurface extraction framework applied to core sample images for dimension reduction of fracture objects 774 . . . . .	28
A mixed-dimensional model for thermo-chemical-flows in fractured porous media 198 . . . . .	30
A modified pulse-decay approach to simultaneously measure permeability and porosity of tight rocks 613 . . . . .	30
A multiscale approach for the characterization of bio-chemo-mechanical processes in con- taminated marine sediments 772 . . . . .	31
A multiscale mixed finite element method applied to the simulation of two-phase flows 730 . . . . .	32
A new discrete fracture model for fluid flow based on phase field method 788 . . . . .	33

A new pore-merging method for simulating mineral dissolution in porous media using pore-network models 279 . . . . .	33
A new probabilistic nucleation model to predict crystal growth in porous medium 236 . .	34
A numerical study on the role of the slight compressibility on viscous fingering 93 . . . .	35
A parallel recursive implementation of the Multiscale Perturbation Method for two-phase flow 591 . . . . .	36
A parallelized method to model combined conductive-radiative heat transfer at local scale within highly porous media 708 . . . . .	37
A phase-field method for propagating fluid-filled fractures coupled to a surrounding porous medium 253 . . . . .	38
A physics-based model to predict the impact of horizontal layers on CO2 plume migration 681 . . . . .	38
A pore-network upscaling framework for the nanoconfined thermodynamic phase behavior in shale rocks 435 . . . . .	39
A poro-elasto-visco-plastic model of the dewatering of a two-phase suspension 209 . . .	40
A posteriori estimates for the Richards equation (nonlinearity, degeneracy & heterogeneity) 171 . . . . .	40
A quantitative study of transition states between single-phase steady flows in a microfluidic device 586 . . . . .	41
A review on the use of microbial induced calcite precipitation for problematic soil engineering 704 . . . . .	42
A sequential grid-block upscaling method for highly heterogeneous tumors: application to osteosarcoma 343 . . . . .	43
A sequential implicit solver for two-phase subsurface flows using the Multiscale Robin Coupled Method 689 . . . . .	44
A space-time multiscale mortar mixed finite element method for flow in porous media 706	44
A stochastic analysis of the non-Newtonian hydraulic behavior of rough fractures 298 . .	45
A theoretical analysis of the nonlinear behaviors in the measurements for two-phase flow in low-permeability core considering the capillary effects 5 . . . . .	46
ANALYTICAL SOLUTION FOR THE POPULATION-BALANCE MODEL DESCRIBING FOAM 168 . . . . .	47
Accelerating Micro-Macro Models for Two-Mineral Reactive Systems with Machine Learning 161 . . . . .	48
Accurate determination of the time-validity of Philip's two-term infiltration equation 766	49
Accurate numerical simulation of electrodiffusion and water movement in brain tissue with cortical spreading depression as a case study 199 . . . . .	50

Adaptive Virtual Element Methods for simulations in Discrete Fracture Matrix models 517	51
Adaptive phase recovery method for three-dimensional porous media reconstruction from its bi-dimensional thin-section 354	51
Additive Manufacturing Via Digital Light Processing of Durable Ceramic Porous Structures for Application to Combustion Systems 88	52
Additive Manufacturing of open porosities: from fabrication and characterization to the application 597	53
Advancements in suction-induced fractures in multiphase porous media: Phase-field and data-driven multiscale modeling 170	54
An Assumed Enhanced Strain (AES) finite element approach in modeling fracture propagation in partially saturated porous media 770	55
An Efficient Solution Strategy for Variational Models of Brittle Fracture 415	55
An adaptively coupled multiphysics model for compositional two-phase flow targeting underground gas storage 106	56
An energy-preserving MAC numerical scheme for the Volume Of Fluid method and application on Taylor flows 360	57
An investigation of drug release from granules linking structure, process and release performance 789	58
An investigation on the accuracy and simulation performance of permeability estimation from 3D pore-scale imaging based on the solution of the Laplace's equation 504	59
An iterative scheme for two-scale phase-field models in porous media. 70	60
An open-source integrated solution for flow and transport in random heterogeneous porous media 151	60
Analysis of droplet mobilization confined in a micro pore-doublet system at low capillary number 519	61
Analysis of the thermal conductance of polymeric ion-exchange membranes 551	62
Analytical Model for Predicting Dynamic Capillary Pressure-Saturation Relationship in Porous Media 244	63
Analytical Modeling of Mass Transfer Integrating Diffusion and Dispersion in Solvent Injection Based Heavy Oil Recovery Methods 624	64
Analytical modelling of foam in porous media 242	65
Analytically Derived Upscaled Relative Permeability Curves for Viscous Limit Flow through Layered Porous Media 599	66
Anomalous nanosilica imbibition in cement-based materials 53	67
Application of Adaptive Conservative Time Integration for Transport in Fractured Porous Media 428	67

Application of Convolutional Neural Networks in Flow Simulation of Porous Media: Unsupervised Image Segmentation and Lat-Net for LBM Simulation 756 . . . . .	68
Application of Helmholtz EDL Theory in a Pore Network Model for Studying Capacitive Deionization 255 . . . . .	69
Application of Lightning Breakdown Simulation in Inversion of Induced Fracture Network Morphology in Stimulated Reservoirs 645 . . . . .	71
Application of the Virtual Element Method to Two-phase Flow of Immiscible Fluids in Porous Media 592 . . . . .	71
Applications of Physics Informed Neural Networks for Modeling Soil Water Dynamics 293	72
Applying Machine Learning Methods to Speed Up Two-Phase Relative Permeability Upscaling 90 . . . . .	73
Applying Reaction-Diffusion Models to Analyse Turing Patterns on Batteries 296 . . . . .	74
Assessment of the role of densification on the displacement of DNAPL in high permeable porous media using a polymer solution 506 . . . . .	74
Assessment of two hydraulic models of canal of Calais regarding the control issue 9 . . . . .	75
Automatic cracks detection in 3D $\mu$ CT images using DVC total variation strain regularization 518 . . . . .	76
Averaged Models for Two-Phase Flow in a Pore: The Effect of Hysteretic and Dynamic Contact Angles 162 . . . . .	77
BDDC for MHFEM discretization of unsteady two-phase flow in porous media 119 . . . . .	78
Bacillus subtilis, A Plant Growth Promoting Rhizobacteria, Improves Soil Hydro-Physical Properties 751 . . . . .	79
Bayesian Inference of Poroelastic Properties from Induced Seismicity Data Using an Energy-based Poromechanics Model 584 . . . . .	79
Benchmark of different coupling schemes for reactive transport in saturated porous media 629 . . . . .	80
Benchmarking Conventional and Machine Learning Segmentation Techniques for Analysis of Digital Rock Physics Properties 33 . . . . .	81
Beyond tortuosity: evaluating connectivity in multimodal catalysis supports 493 . . . . .	82
Block Copolymer Ultrafiltration Membranes: Stochastic Microstructure Delineation and Flow Simulation 819 . . . . .	83
Block-partitioned solvers for poromechanics via gradient flows and minimization 596 . . . . .	83
Bounds for effective Forchheimer coefficient in randomly heterogeneous porous media 684	84
Bulk and interfacial properties of alkanes in the presence of carbon dioxide, methane, and their mixture 243 . . . . .	85
CCSNet: a deep learning modeling suite for CO <sub>2</sub> storage 423 . . . . .	86

COUPLING FREE FLOW AND POROUS-MEDIUM FLOW: COMPARISON OF NON-REFINED, GLOBALLY-REFINED AND LOCALLY-REFINED AXIPARALLEL FREE-FLOW GRIDS 37 . . . . .	87
CPG modelling in fluvial channelised systems under uncertainty 149 . . . . .	88
CT histogram-based estimation of sub-resolution porosity of sintered lunar regolith simulant 155 . . . . .	88
Calcite dissolution in crude oil and formation of crystals on surface of Mica during Ageing Process 805 . . . . .	89
Calculation Studies on Miscibility Characteristics of the CO <sub>2</sub> /n-Hexadecane System with Presence of Water Component under Geological Conditions 179 . . . . .	90
Calculation of relative permeabilities for two-phase flows in highly permeable porous media: direct calculation vs. closure problems 574 . . . . .	91
Capillary imbibition dynamics under various solid–liquid interactions: A molecular dynamics study 609 . . . . .	92
Capillary pumping: a transport mechanism in partially wet porous networks 716 . . . . .	93
Capsule-based biomimetic regulating technique of MICP and its application for soil reinforcement 771 . . . . .	93
Cell-scale haemodynamics and transport in canonical disordered porous media: numerical simulation and microfluidic experiments 610 . . . . .	94
Characterising multi-domain porous structure of the human placenta by synchrotron X-ray micro-tomography 602 . . . . .	95
Characterization of microbial distribution of packaging material processes over a production cycle 640 . . . . .	96
Characterization of wettability control on dynamics of two phase flow in natural porous media 288 . . . . .	97
Clay settling in fresh and salt water: new dynamic X-ray micro-CT insights 478 . . . . .	98
Coal Relative Permeability Measurements Using Lab-on-a-chip Method 137 . . . . .	99
Coffee is for drinking, tea is for porous media science: intermittent burst dynamics in slow drainage experiments in porous media 492 . . . . .	100
Comparative study on oil recovery efficiencies of ScCO <sub>2</sub> and N <sub>2</sub> injection processes in tight cores 183 . . . . .	101
Comparison Modified Method of Peng-Robinson Equation of State in the Process of Gas Injection of Nanopores 256 . . . . .	102
Comparison and Reduction of the Chemical Kinetic Mechanisms Proposed for Thermal Partial Oxidation of Methane (TPOX) in Porous Media 802 . . . . .	103
Comparison of Response Surface and Artificial Neural Network Model for Relative Permeability using Saturation and Phase Connectivity 749 . . . . .	103



Comparison of mechanical and hydro-mechanical models for rough fracture closure 665 . . . . .	104
Compositional modeling in porous medium using iterative IMPEC scheme and constant volume-temperature flash 430 . . . . .	105
Computational analysis of Single- and Two-Phase Flow with Poroelasticity 441 . . . . .	105
Computational modeling based on decomposition methods applied to polymer flooding in oil reservoir 608 . . . . .	106
Conceptual model of reactive transport incorporating with dynamic biofilm growth and multicontinuum media 432 . . . . .	107
Cone beam computed tomography reconstruction for digital rock 222 . . . . .	108
Control of chemically-driven convective dissolution by differential diffusion effects 731 . . . . .	109
Controlling Gas Diffusion Layer Wettability via Additive Manufacturing and Simulation 39	110
Controlling viscous fingering in hierarchal porous media 240 . . . . .	111
Converging gravity currents of power-law fluids in the subsurface 583 . . . . .	111
Correctors and error estimates for reaction-diffusion processes through thin heterogeneous layers 284 . . . . .	112
Coupled LBM-MHFEM simulator for vapor transport in air over a moist soil layer 400 . . . . .	113
Coupled Thermal-Hydrological-Mechanical-Chemical Model For Reactive Dissolution and Wormhole Formation in Vugs Carbonate Rocks 49 . . . . .	114
Coupled Thermal-Hydrological-Mechanical-Chemical Model For Reactive Dissolution and Wormhole Formation in Vugs Carbonate Rocks 246 . . . . .	115
Coupled flow and deformation in heterogeneous fractured media: A multirate mass transfer approach for double-porosity poroelasticity 532 . . . . .	116
Coupling strategies for free flow with porous media -from single to two phase flow- 156 . . . . .	117
Data assimilation for reducing uncertainty of subsurface flow modeling using meshless method 92 . . . . .	117
Data driven analysis of evapotranspiration estimated by the water balance and eddy covariance methods 662 . . . . .	118
Data-Driven Finite Element Method, Energy Conservation approach for temperature, water isotope ( $\delta D$ , $\delta^{18}O$ ), and $[SiO_2]_{sat}$ . conc. distributions of the Culex Basin terrestrial hydrothermal system-Yellowstone, WY. 627 . . . . .	119
Data-based prediction of transport in heterogeneous porous media 809 . . . . .	120
Deep Learning-based sensitivity analysis for subsurface flow and transport 580 . . . . .	121
Deep learning enhancement of micro-CT images for large-scale flow simulation 83 . . . . .	121
Deep learning for digital rock image segmentation in pore structure characterization 133	122

Deep-learning-based Image Segmentation Techniques for Porous Media Property Estimation 701 . . . . .	123
Deep-learning-based surrogate model for brine extraction well placement for geological carbon storage 391 . . . . .	124
Deformation-driven solute transport in soft porous media 456 . . . . .	124
Density instabilities due to evaporation from porous media 181 . . . . .	125
Determination of Characteristic Transport Coefficients of Porous Media: A Diffuse Interface approach 604 . . . . .	126
Developed emulsification in porous media flow 394 . . . . .	126
Development of a new complex fluid for DNAPL recovery and nZVI delivery 479 . . . . .	127
Development of a simple-to-use and novel correlation to predict apparent viscosity of waxy crude oils mixed with polymeric additives 176 . . . . .	128
Development of flow through cell method for in-situ visualization of dissolution processes in solid dosage forms 533 . . . . .	129
Diffusion of water in palm leaf materials 734 . . . . .	130
Digital Rock Analysis of Low Resistivity Pay Zones to Refine Saturation 7 . . . . .	131
Digital Rock Typing 636 . . . . .	132
Digital rock approach for unconsolidated sandpacks using pore network modelling: comparison between experiments and simulations 175 . . . . .	132
Direct Pore-scale Simulation of Thermal-Hydraulic-Mechanical Coupling Effect on the Process of Waterflooding with FVM Method 154 . . . . .	133
Direct Visualization of Induced Asphaltenes Removal in Carbonate Rock Using Confocal Imaging 347 . . . . .	134
Dispersive effects in buoyancy-driven flow including plume-fed gravity currents 307 . . . . .	134
Dissolution and swelling in porous media 300 . . . . .	135
Does the imaging domain size matter in modeling the permeability of bioclogged porous media inside a microfluidic channel with evolving biofilms? 727 . . . . .	136
Droplet absorption into thin layers of hydrogel 712 . . . . .	137
Droplet formation, growth and detachment on the interface of a coupled free flow – porous medium system 180 . . . . .	137
Drying of capillary porous media simulated by coupling of continuum model and pore network model 15 . . . . .	138
Drying of cellulose studied by Nuclear Magnetic Resonance 221 . . . . .	139
Dynamic adsorption of CO <sub>2</sub> in shale organic pores using molecular dynamic simulation 263 . . . . .	139

Dynamic coarsening for efficient simulation of geothermal energy applications 638 . . . . .	140
Dynamic imaging of the impacts of flow instabilities and rock heterogeneity on CO <sub>2</sub> plume migration 85 . . . . .	140
Dynamic mesh optimisation for geothermal reservoir modelling 366 . . . . .	141
Dynamic pore-network modeling of coupled compositional flow and phase change dynamics in porous media 436 . . . . .	142
Dynamics of Water and Gas Injection in an Oil-Wet Reservoir Rock at subsurface conditions: A Pore-Scale Synchrotron X-ray Imaging Study 78 . . . . .	143
Dynamics of organic pore evolution in shale under varying thermal and oxygen environments 289 . . . . .	144
Dynamics of unsaturated flow in fracture networks: impact of local splitting behavior at the intersection 697 . . . . .	145
EPISODIC EXTREME RAINFALL EVENTS DRIVE GROUNDWATER RECHARGE IN ARID ZONE ENVIRONMENTS OF CENTRAL AUSTRALIA 184 . . . . .	146
EUTROPHICATION CONTROL TREATMENTS AND SEDIMENT POROSITY 282 . . . . .	146
EVALUATION OF SURFACTANT AND FOAM PROCESSES FOR IN-SITU NAPL REMEDIATION IN A MILITARY BASE, SOUTH KOREA 62 . . . . .	147
EXPERIMENTALLY VALIDATED SIMULATION OF STRAIN-INDUCED BATTERY AGING 38 . . . . .	148
Effect of Pore-Scale Wettability Distribution Patterns on Fluid Connectivity 118 . . . . .	149
Effect of The Relative Humidity on The Porosity of PEM Fuel Cell Catalyst Layers 464 . . . . .	150
Effect of Viscosity Contrast on Miscible Rayleigh-Taylor Convection in Porous Media 72 . . . . .	151
Effect of Wettability on Immiscible Liquid Displacement in 2D and 3D Porous Media 295 . . . . .	151
Effect of grain circularity on the temporal evolution of interfacial area 557 . . . . .	152
Effect of grain shape on quasi-static fluid-fluid displacement in porous media 148 . . . . .	153
Effect of non-uniform passive advection on A+B->C radial reaction-diffusion fronts 692 . . . . .	153
Effect of pore geometry and contact angle on the capillary pressure and oil recovery factor in models of porous media 373 . . . . .	154
Effect of surfactants on liquid absorption into porous media 144 . . . . .	155
Effective Transport Parameters of Porous Media from Microstructure Images. 593 . . . . .	155
Effective dispersion coefficients for the upscaling of pore-scale mixing and reaction in heterogeneous porous media 745 . . . . .	156
Effects of Inertia and Diffusion on Reactive Transport with Fluid-Solid Reactions in Rough Fractures 292 . . . . .	157

Effects of Soil Heterogeneity and Transient Flow on Multicomponent Biodegradation 725	158
Effects of nanopore geometry on confined water flow: a view of lattice Boltzmann simulation 73	159
Efficient Numerical Design of Porous Materials With Target Properties and Microstructure 818	159
Efficient methane gas production strategies from gas hydrate reservoir using the numerical simulations 764	160
Elastic turbulence generates anomalous flow resistance in porous media 228	161
Elasticity of argon in nanopores of different sizes 211	161
Electrical Impedance Spectroscopy: a tool to investigate interactions between complex fluids – porous materials 146	162
Electrokinetic delivery of reactants in porous media: solution chemistry controls transport, mixing and degradation 323	163
Energy dissipated through Haines jumps in disordered media 447	164
Energy dissipation as heat in porous media flow 8	164
Enzymatic degradation of biomass: a porous media approach 190	165
Estimation of auto-covariance of log hydraulic conductivity from Generalized sub-Gaussian porosity and particle size random fields 509	166
Estimation of unsaturated soil hydraulic properties by integrated hydrogeophysical inversion of time-lapse ground-penetrating radar measurements 647	167
Evaluating the interaction of biofilms, organic matter and soil structures at the pore scale 547	168
Evaluation of mineral surface area evolution during dissolution reactions 297	169
Evaluation of the Impact of Flow Field Design on the Porosity of Zinc Deposition in the Zinc-Iodide Flow Battery by X-ray Computed Tomography 460	169
Event-based measurements of contact angles during imbibition to evaluate contact angle hysteresis on a pore-by-pore basis using micro-CT 107	170
Evolution of Bentheimer Sandstone Wettability During Cyclic scCO <sub>2</sub> -Brine Injections 643	171
Evolution of fracture permeability induced by THMC-coupled processes 77	172
Examining the Structure of Supercritical CO <sub>2</sub> using X-ray Raman Spectroscopy and Atomistic Scale Modeling 387	173
Experimental Determination of Intrinsic In-Plane Permeability for Thin Porous Media 429	173
Experimental Evaluation of Polymeric Fluid Displacement in Carbonates using an X-ray Imaging Technique 280	174

Experimental Investigation of Capillary Number's Control on Stress-Dependent Shifts in Irreducible Saturation in Deformable Porous Media 444 . . . . .	175
Experimental Study on Long Core of Fractured Vuggy Metamorphic Rock Rich in Condensate Gas Reservoir with Different Development Methods 523 . . . . .	176
Experimental analysis and modeling of non-isothermal transient flows in granular porous media at large Biot numbers 792 . . . . .	177
Experimental and Numerical Study of the Dynamic Wetting influence on the Multiphase Flow in a Pore Doublet Model 485 . . . . .	178
Experimental investigation of buoyant convection in a heterogeneous porous media: Two-layers separated by an inclined permeability jump* 173 . . . . .	178
Experimental investigation of physical dispersion and in-situ mixing during low salinity waterflooding 81 . . . . .	179
Experimental study of drying in the presence of fluorescent colloidal particles in model porous media 570 . . . . .	180
Experimental study of steady state flow paths during the immiscible flow of ganglia in stochastic porous media micromodels 653 . . . . .	181
Experimental study of the contact angle of hydrogen-brine-rock for subsurface energy storage 227 . . . . .	182
Experimental study of water vapour condensation in cracked concrete with different specimen states visualised by neutron tomography 372 . . . . .	183
Explicit simulation of seismic waves in fluid-filled fractured porous media 46 . . . . .	184
Extending a low permeability fluid flow model for transient flow of compressible and slightly compressible fluids. 820 . . . . .	185
Extending equilibrium thermodynamics to include fluid-surface interaction for nanonconfined fluids 484 . . . . .	186
Extension of SAFT equation of state to include calcite wall effect in water properties within water-calcite interface using molecular dynamic simulations 195 . . . . .	186
FEM Modeling of Spherical Indentation in a Poro-elasto-plastic Medium 775 . . . . .	187
FLEXT – A Flexible Scripting X-ray Computed Tomography System for Multiscale and Dynamic Imaging of Porous Materials 723 . . . . .	188
Fabrication of Reactive Rocks with 3D Printing 562 . . . . .	189
Fault permeability and rupture in injection-induced earthquakes 245 . . . . .	189
Feedback mechanisms between precipitation and dissolution reactions across randomly heterogeneous conductivity fields 571 . . . . .	190
Film entrainment and particle transport during gas invasion in suspension-filled microchannels 548 . . . . .	191
Filtration with multiple species of particles 421 . . . . .	192

Fixed Stress Splitting for Coupled Flow and Poromechanics 224 . . . . .	192
Flow behavior in a rough channel with pore scale simulation 34 . . . . .	193
Flow in deformable fractures - From numerical studies to experimental investigations 124	193
Flow instabilities of viscoelastic polymer solutions in multiple contraction channels 568 .	194
Flow of DNA solutions around cylindrical arrays 737 . . . . .	195
Flow patterns and interface stability during drainage of liquid-particle mixtures 241 . . .	195
Flow rate and dissolution rate Impacts on the wormhole formation 114 . . . . .	196
Fluid charging and hydrocarbon accumulation in the sweet spot, Ordos Basin, China 74 .	197
Fluid flow control devices with 3D-graded permeability 250 . . . . .	197
Fluid rearrangements during Haine's jumps using time-resolved micro-computed tomog- raphy 588 . . . . .	198
Fluid-Fluid Displacement in Mixed-Wet Porous Media 60 . . . . .	199
Fluid-driven particle transport patterns in fractures 535 . . . . .	200
Fluid-fluid phase separation in a soft porous medium 569 . . . . .	201
Fluid-solid interfacial area at different wetting conditions during multiphase in a porous medium 762 . . . . .	201
Fluid-structure interactions in a soft-walled Hele-Shaw cell 281 . . . . .	202
Flux Regression Performances of Deep Learning in Discrete Fracture Networks 324 . . .	203
Forced air and water flow in granular media – models and experiments 55 . . . . .	203
Free flow over porous media: Heterogeneity and the Beavers-Joseph interface condition 739 . . . . .	204
From the non-linear Darcy law for immiscible two-phase flow in porous media to constitu- tive equations for each fluid species 20 . . . . .	205
GMsFEM for Reduced Model of Darcy Flow in Fractured Porous Media 302 . . . . .	206
Gas shale swelling and shrinkage characterized by controlled suction experiments 252 . .	206
Gas water two phase flow in fractured-porous carbonates 96 . . . . .	207
Gas-liquid phase separation in a soft porous medium 483 . . . . .	208
Generalized coupling conditions for arbitrary flows to the fluid-porous interface 434 . . .	209
Generating unrepresented geological realizations using Generative Adversarial Networks 667 . . . . .	209
Generation of Virtual Nonwoven Structures and Simulation Studies of Compression Behav- ior and Flow Permeability 459 . . . . .	210

Geometry evolution and fracture alteration controlled by spatial mineral heterogeneity during CO <sub>2</sub> sequestration – A reactive transport study 313 . . . . .	211
Geostatistical Inversion in Geologic CO <sub>2</sub> Sequestration Using a Variational Autoencoder 521 . . . . .	212
Glass Micromodels Study of Emulsified Polymer Gel System for Conformance Control Applications 424 . . . . .	212
Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions 718 . . . . .	213
Global random walk solvers for flow and multi-component reactive transport in heterogeneous porous media 660 . . . . .	214
Global sensitivity analysis of a low permeability media gas flow model with multiple transport mechanisms 322 . . . . .	215
Graded viscosity banks on the rear end of the polymer slug 294 . . . . .	216
Gradient discretization of two-phase flows coupled with mechanical deformation in fractured porous media 67 . . . . .	216
Graphene oxide nanoparticles for aquifer remediation: transport experiments and reactivity batch tests. 765 . . . . .	217
Gravitational instabilities in a 2D porous medium for carbon dioxide sequestration 577 . . . . .	218
Gravity-driven instability in fracture flows with miscible fluids of different densities 384 . . . . .	220
Growth and upscaling of viscous fingers in immiscible two-phase flow 383 . . . . .	220
Growth of gas-filled penny-shaped cracks in decompressed hydrogels 714 . . . . .	221
HYDRUS and analytical modeling of seepage in porous banks of commingled ephemeral streams having triangular flash-flood hydrographs: emergence and extinction of an “ephemeral” unconfined aquifer 178 . . . . .	222
Heat and mass transfer in a shear-thinning fluid through porous media 188 . . . . .	223
Heterogeneity Evaluation of Microstructures in a Sandstone Reservoir Using Micro-CT Imagery 489 . . . . .	224
Heterogeneity effects on the Solubility-trapping during CO <sub>2</sub> Geological Sequestration 555 . . . . .	225
Heterogeneous Wettability in Porous Catalyst Layers of PEM Fuel Cells: Modeling-based Analysis and Design 321 . . . . .	226
High Speed-Laser Speckle imaging to unravel pico-liter droplets substrate interactions 340 . . . . .	227
High-order ADE solution for the fluid diffusion equation and application in coupled hydro-mechanical simulation 111 . . . . .	228
Higher-Order Finite Element Multiphase Multicomponent Reactive Transport Model for Unstructured and Fractured Grids 375 . . . . .	228

Hindered thermally driven migration of a drop on a chemically patterned wall chemically patterned solid wall 450 . . . . .	229
Homogenization approach to the upscaling of a reactive flow through particulate filters with wall integrated catalyst 457 . . . . .	230
Homogenization of Flow in Porous Media with Isolated Embedded Fractures 101 . . . . .	231
Homogenization of the linearized ionic transport equations in random porous media 259	231
Homogenization of two-phase flow in porous media: A diffuse interface approach explaining capillary pressure-saturation hysteresis 336 . . . . .	232
How Harry Vereecken's work contributes to reach the 2030 global sustainable development goals. 399 . . . . .	233
How do plants transport water under negative pressure? 794 . . . . .	234
How does the power law dependency of flow rate on pressure gradient when viscous and capillary forces compete, scale with system size? 19 . . . . .	234
How does the structure of a gas diffusion layer control the performance of fuel cells 32 .	235
How heterogeneous distributions of wettability affects infiltration into soil 474 . . . . .	236
How to capture centimeter-scale local variations in the pore space of paper: A benchmark study using $\mu$ -CT 217 . . . . .	236
Hydrate formation and migration in stratified porous media 524 . . . . .	237
Hydraulically driven fractures in deformable porous media- Impact of non-linear flow patterns in vicinity of fractured zone 496 . . . . .	238
Hygromechanical Properties of PEG-Treated Archaeological Wood: Molecular Simulation and Poromechanics 603 . . . . .	239
Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis: Role of components, interphases and hydrogen bonding 605 . . . . .	240
Ice crystallization and mechanical damage at the pore scale 488 . . . . .	241
Identification of transport and clogging parameters of porous media 268 . . . . .	242
Image Segmentation with Transfer Learning for Carbonate Rock Images 136 . . . . .	243
Image-based modeling of spontaneous imbibition in porous media 539 . . . . .	244
Image-based morphological characterization of multiphase porous media flow 469 . . . . .	244
Imbibition Effect and Driving Mechanism of Nanofluid in Porous media 688 . . . . .	245
Imbibition-Induced Deformation in Nanoporous Vycor Glass 451 . . . . .	246
Impact of Multi-scale Deformations on Multiphase Flow Considerations in Porous Media 793 . . . . .	247
Impact of Physical Heterogeneity on Effective Reaction Rates 301 . . . . .	247



Impact of Roughness on Multiphase Fracture Flow - Insights from 3D-Printed Fractures	112 248
Impact of Wettability on Reservoir Quality Distribution and Preservation	717 . . . . . 249
Impact of operational factors on Aquifer Storage and Recovery (ASR) scheme in saline regions	810 . . . . . 249
Impact of osmosis and emulsification on oil remobilization in pore-scale experiments	158 250
Impact of pore-space variations and orientation of layering on the flow properties of Coquina limestone	269 . . . . . 251
Impact of salt on sorption isotherms in nanoporous media	351 . . . . . 252
Implementation of Higher-Order methods for Modeling of the Single-Phase Multicomponent Flow in Porous Media	462 . . . . . 252
Implications of plant exudates on the formation of rhizosheaths	817 . . . . . 253
Improved Watershed-based Pore Space Partitioning Algorithm for Pore Network Modelling	86 . . . . . 254
Improved micro-continuum formulations for pore-scale simulation of mineral dissolution	404 . . . . . 254
Improvements of stochastic simplex approximate gradient (StoSAG) for production optimization	674 . . . . . 255
Improving the accuracy of multiscale methods with informed interface spaces based on physics	693 . . . . . 255
Improving the reliability of phase segmentation by combining 3D imaging and machine learning methods	694 . . . . . 256
In situ study of 3D fluid fingering in porous media using X-ray Computed Tomography	673 257
In-Situ Micro-CT Studies to Understand the Role of Salt Precipitation during CO <sub>2</sub> Storage in Saline Aquifers	461 . . . . . 258
In-situ real-time imaging to characterize spatially heterogeneous calcite dissolution rates at the nanoscale	449 . . . . . 259
Incompressible Smoothed Particle Hydrodynamics as a tool for modelling electrolyte distribution in Gas Diffusion Electrodes	471 . . . . . 259
Influence of intermittency effects on anomalous transport in single- and multi-phase flow in porous media	754 . . . . . 260
Initial estimation of field-scale macropore parameters for use in dual-permeability models	344 . . . . . 261
Injectivity Decline by Nanoparticles in High Permeability Sandstone Rock	690 . . . . . 262
Inkjet printing lines onto thin, moving porous media - experiments	121 . . . . . 263
Inkjet printing lines onto thin, moving porous media - simulations	122 . . . . . 264

Insights from reactive percolation experiments on the geological storage of CO <sub>2</sub> in natural serpentinites 710 . . . . .	264
Insights into capillary pressure in the GDL of operating polymer electrolyte fuel cells 741	266
Integrating Machine Learning into a Methodology for Early Detection of Wellbore Failure 779 . . . . .	266
Integrating process-based reactive transport modeling and machine learning for surrogate model development: an application to electrokinetic remediation of contaminated groundwater 319 . . . . .	267
Inter-well Connectivity Analysis and Productivity Prediction Based on Intelligent Connectivity Model 617 . . . . .	268
Interaction Problems between Fluids and Poro-Elastic Media - Applications in Life Sciences 352 . . . . .	269
Interaction of Nanoparticles and Surfactant in Controlling Foam Stability 329 . . . . .	269
Intermediate-scale testing of a spatially distributed sensing technology for monitoring gas emission from soils as applied to climate change 791 . . . . .	270
Introduction of Anisotropic Heat Transfer Coefficient 353 . . . . .	271
Introduction of an Integrated Workflow for Optimal Well Placement Using Machine Learning Methods 267 . . . . .	272
Inverse modeling of transient three-dimensional core-scale two-phase flows 649 . . . . .	273
Investigating signatures of fracture evolution during the drying of clay-rich architected porous media 761 . . . . .	274
Investigating the Effect of Enzymatically Induced Carbonate Precipitation on Hydraulic Properties 680 . . . . .	275
Investigating the Influence of Non-Linear Interfacial Partitioning on Aqueous Film Forming Foam (AFFF) Transport and Retention in the Unsaturated Zone 683 . . . . .	275
Investigation of Emulsion Flow in Microfluidic Fracture with Varying Aperture 607 . . . . .	276
Investigation of species transport in fractured media using 3D printed micromodels 631 . . . . .	277
Investigation on multi-scale pore seepage model of shale gas reservoir considering diffusion and slippage effect 536 . . . . .	278
Lab-scale characterization of a shaly caprock for CO <sub>2</sub> storage: advancements and limitations 103 . . . . .	279
Laboratory scale investigation of CO <sub>2</sub> flow mechanisms across clay-rich caprock 439 . . . . .	280
Lagrangian Intermittency in Colloid Transport Through Porous Media 440 . . . . .	280
Lamellae Generation and Dynamics During Gas Invasion of a Porous Medium Occupied by a Surfactant Solution 368 . . . . .	281

Lattice Boltzmann modeling of contact angle hysteresis in liquid drying in porous media 403 . . . . .	282
Lattice Boltzmann simulation in the context of battery systems 398 . . . . .	282
Lattice Boltzmann simulations of invasion in porous transport layer (PTL) at anode side of polymer electrolyte membrane (PEM) water electrolyser 40 . . . . .	283
Life in a tight spot: How bacteria move in porous media 367 . . . . .	284
Linearized Water and Air Flow in Porous Media 56 . . . . .	285
Linking DFT and MD to simulate grand canonical ensemble: selectivity of binary mixtures in nanopores 283 . . . . .	286
Linking processes, scales, and research communities to advance research on the most im- portant porous medium we have: our Earth. 410 . . . . .	287
Long-term redistribution of residual gas due to non-convective transport 396 . . . . .	288
Long-time shadow limit for a reaction-diffusion-ODE system 641 . . . . .	289
Lubricated hydrodynamic interactions between a hard spherical indenter and a poroelastic nanolayer 370 . . . . .	289
MATBOX, an Open-Source Microstructure Analysis Toolbox for Meshing, Generation, Seg- mentation, and Characterization of 3D Heterogenous Volumes 210 . . . . .	290
MOFs based CH <sub>4</sub> Hydrate Formation and Self-Preservation 452 . . . . .	291
Machine learning prediction of Lennard-Jones fluid self-diffusion in pores 564 . . . . .	292
Macroscopic model for flow in exuding porous media 514 . . . . .	292
Magnetic Resonance Imaging of Fluid Compositions in CO <sub>2</sub> Displacement of Decane in Berea Sandstone 695 . . . . .	293
Magnetic Resonance and Magnetic Resonance Imaging of Porous Media – Recent Develop- ments 646 . . . . .	294
Magnetic resonance imaging of water content and flow processes in natural soil using pulse sequences with ultrashort detection 328 . . . . .	295
Manufacturing of polycrystalline nickel-based superalloy membranes by directional coars- ening through rolling and ageing 498 . . . . .	296
Mapping Land Use and Land Cover Changes in Gilan Province of Iran between 1975 and 2015: GIS and Remote Sensing Analyses 115 . . . . .	297
Marangoni Effect Reshapes Drying Pattern in Porous Media 516 . . . . .	298
Material balance and mixing behavior during emulsification of crude oil by using micro-X- ray tomography 393 . . . . .	299
Mathematical Modeling of the Effect of Acoustic Waves on oil Recovery in Porous Media 346 . . . . .	299

Measuring The Anisotropic Heat Transfer Coefficients In Carbon Fiber Felt 226 . . . . .	300
Measuring and modelling multi-scale fluid distributions in heterogeneous rocks based on X-ray micro-computed tomography 102 . . . . .	301
Measuring co-diffusion kinetics on thin films 825 . . . . .	302
Mechanisms of gas separation through 2D porous graphene membranes : theory and molecular simulations 481 . . . . .	302
Meshless Lattice Boltzmann Method for pore-scale porous media flow 196 . . . . .	303
Mesoporous, Moisture-Absorbent, Temperature-Controlled Hydrogels For Atmospheric Water Harvesting 169 . . . . .	304
Mesoscale Modelling of Thermal-Chemical processes during Nuclear Fuel Corrosion 16 . . . . .	304
Mesosopic modeling of porous media with application to electrochemical energy conversion and storage devices: the case of gas diffusion layers and proton-exchange membranes 185 . . . . .	305
Methane adsorption on Silica-Kaolinite interface for shale gas application: A theoretical study 314 . . . . .	306
Method for predicting a reasonable water injection pressure for a fractured low-permeability sandstone reservoir 534 . . . . .	307
Micro-macro Modeling Approaches for Reactive Multiphase Flow and Transport in Complex Media 276 . . . . .	308
Micro-scale Insights into the Effects of Ionic Strength on CO <sub>2</sub> Induced Carbonate Rocks Dissolution 552 . . . . .	309
Microbial Induced Desaturation and Precipitation (MIDP) in Stratified Granular Soil 420 . . . . .	310
Microfluidic and numerical investigation of recirculation induced reaction hot spots in a porous media analog 412 . . . . .	310
Microfluidic investigation of phase banking during low tension displacements 782 . . . . .	311
Microscale modeling of thermo-hydro-mechanical behavior of fruit tissue during drying 786 . . . . .	312
Microstrokes and capillary dilations – investigating the effect of single capillary alterations 316 . . . . .	313
Microstructural Evolution of Sand Assembly in Direct Shear Test: An Experimental Study using X-Ray Tomography 615 . . . . .	314
Microstructure changes of oilwell cement enhanced by micro crystalized Ca-montmorillonite in ScCO <sub>2</sub> condition 526 . . . . .	315
Mineral reaction and salt precipitation on a chip: understanding aquifer-relevant geological processes during CO <sub>2</sub> injection 389 . . . . .	315
Mineralisation from carbon dioxide convective dissolution in a packed bed Hele-Shaw reactor 748 . . . . .	316

Modeling capillary fluctuations for fluid flow with lattice Boltzmann methods using LBPM 709 . . . . .	317
Modeling coupled porous media/free flow/drop interaction in a PEM fuel cell using a pore- network approach 80 . . . . .	318
Modeling lithium diffusion in battery cathodes considering chemo-mechanically induced damage 497 . . . . .	319
Modeling of the droplets capture/release dynamic of Water-Alternated-Emulsion flooding in porous media through a non-equilibrium mass transfer. 220 . . . . .	319
Modeling on contaminants removal by foam with nanoparticles in heterogeneous porous media 501 . . . . .	320
Modeling rate-dependent relative permeability of three-dimensional heterogeneous struc- tures with a one-dimensional semi-analytical approach 59 . . . . .	321
Modeling the evolution of fractured media using a multiscale approach 622 . . . . .	322
Modeling the force balance controlling spatial distribution of deposited polymeric sub- stances in porous media 480 . . . . .	323
Modeling transport of methane under nanoconfinement and in complex geometries using LBM 127 . . . . .	324
Modelling Multi-scale 3-D Digital Rocks by a New Image Segmentation Method 335 . . .	324
Modelling and analysis of multicomponent transport at the interface between free and porous-medium flow influenced by radiation and roughness 145 . . . . .	325
Modelling dynamic behavior of an infiltration trenches system 249 . . . . .	326
Modelling hydrate formation in porous media: Capillary inhibition effects 350 . . . . .	326
Modelling pressure-saturation curves that exhibit hysteresis and forced imbibition with the pore-morphology method 468 . . . . .	328
Modelling rhizosphere water movement in whole plant models 711 . . . . .	329
Modelling the role of vWF in initiating arterial thrombosis 333 . . . . .	330
Modification method and adaptability of fluid phase states in nanopores 823 . . . . .	331
Modification of Darcy's Law by Considering the inertial effect 755 . . . . .	332
Molecular Dynamics Study on Coal Matrix Swelling Characteristics by CO <sub>2</sub> , N <sub>2</sub> , and CO <sub>2</sub> - N <sub>2</sub> Mixture 639 . . . . .	332
Molecular dynamics study of methane diffusion in flexible microporosity of source rock's organic matter 348 . . . . .	334
Multi-parameter Screening Study on Static Properties of Nanoparticle Stabilized Supercrit- ical CO <sub>2</sub> Foam 238 . . . . .	334
Multi-phase flow parameters for unconsolidated reservoirs using digital rock physics 395	335

Multi-scale dynamics of colloidal deposition and erosion in porous media 247 . . . . .	336
Multi-scale imaging and modelling for reactive diffusion at the pore scale 702 . . . . .	337
Multilayered poroelasticity interacting with Stokes flow 28 . . . . .	337
Multiphase imbibition dynamics in xylem-like nanoporous media 349 . . . . .	338
Multiphysics modeling of vanadium redox flow batteries. 214 . . . . .	338
Multiscale Model Reduction of Thermoporoelasticity Problems in Heterogeneous and Frac- tured Media Using Generalized Multiscale Finite Element Method 528 . . . . .	339
Multiscale Modeling of Direct Contact Membrane Distillation: Macroscopic Modeling and Pore Scale Modeling 507 . . . . .	340
Multiscale Sampling for Subsurface Characterization 578 . . . . .	341
Multiscale modeling and simulation of microbially-induced calcite precipitation in porous media 531 . . . . .	342
Multiscale pore network modeling of a carbonate rock sample using micro-CT and SEM images 409 . . . . .	343
Nano-scale wetting film impact on multiphase transport properties in porous media 595 .	344
Nanofluid Evaluation for Enhanced Oil Recovery 816 . . . . .	345
Near-term forecasts of soil water states 418 . . . . .	346
Non-Newtonian flow in macroscopic heterogeneous porous media: from power-law fluids to rheology with change of behavior 317 . . . . .	347
Non-destructive 3D mapping of mineral composition and clay mineral orientation in shale 575 . . . . .	347
Non-intrusive reduced order modeling of natural convection in porous media 503 . . . .	349
Non-invasive characterization of soils and aquifers: 20 years of hydrogeophysics at the Agrosphere institute 446 . . . . .	350
Non-solvent Induced Phase Separation: A Synthetic Approach Towards High Performance Redox Flow Battery Electrodes 565 . . . . .	350
Non-thermal Fluctuations in Stead-State Multiphase Flow in Porous Media 22 . . . . .	352
Numerical Modeling for the Reactive Process of Thermochemical Energy Storage Based on Lattice Boltzmann Method 134 . . . . .	353
Numerical Modeling of Capillary-Driven, Paper-Based, Flow-Through, Microfluidic Redox Flow-Batteries 91 . . . . .	353
Numerical Simulation of CO <sub>2</sub> Huff-n-Puff to Enhance Oil Recovery from Tight Oil Reser- voirs. A Case Study. 633 . . . . .	354
Numerical Simulation of Coupling Darcy and Forchheimer Flow in the Carbonate Reservoir 651 . . . . .	355

Numerical modeling to optimize nitrogen fertigation with consideration of transient drought and nitrogen stress 448 . . . . .	356
Numerical modelling and experimental validation of percutaneous vertebroplasty 676 . . . . .	356
Numerical modelling workflow for the assessment of long term CO2 storage in saline aquifers using the Sleipner dataset 229 . . . . .	357
Numerical scheme for a coupled system in geomechanics 299 . . . . .	358
Numerical simulation aiding the development of superhot geothermal resources 812 . . . . .	358
Numerical simulation of EGS thermal recovery in Multi-stage Hydraulic Fractured Horizontal Wells 445 . . . . .	359
Numerical simulation of slope failure in a gas hydrate-bearing continental slope 27 . . . . .	360
Numerical studies of capillary flow in paper-based microfluidic devices 560 . . . . .	360
Numerical study of dispersion through displacing phase in unsaturated porous media 658 . . . . .	361
Numerical study of the temperature effects on MICP 194 . . . . .	362
Numerical yield surface determination of cemented rocks from digital microstructures 433 . . . . .	363
OPTIMUM SEGMENTATION OF A SANDSTONE RESERVOIR MICRO-CT IMAGERY USING MACHINE LEARNING ALGORITHMS 495 . . . . .	363
Oil Displacement by Water Through an Ultra-Narrow Kerogen Pore Throat: a Molecular Dynamic Study 248 . . . . .	364
Oil recovery mechanisms in fractured tight carbonates by low-IFT foams 425 . . . . .	365
On Fuzzy-Systems Modeling of Subsurface Flow 721 . . . . .	366
On Modeling Nonlinear Flow and Reactive-Diffusion Processes in Heterogeneous Fractured-Porous Media 31 . . . . .	366
On a coupled FE-formulation for the freezing process of ice within the framework of the TPM 453 . . . . .	367
On compressibility error of the lattice Boltzmann method for pore scale modeling of non-Darcy flow 719 . . . . .	368
On pore scale simulation of reactive flows in the case of complex catalytic reactions 699 . . . . .	368
On predicting pore fluid pressure changes in unsaturated porous media subject to undrained processes 76 . . . . .	369
On the Equations of Nonlinear Single-Phase Poroelasticity 193 . . . . .	370
On the effects of colloidal particles in controlled oil-water interfaces. 589 . . . . .	370
On the inverse problem of identifying the effective pore size distribution using non-Newtonian fluids 408 . . . . .	371

On the mechanical behavior of expansive porous media with consideration on chemical effects 75 . . . . .	372
On the value of using electrical resistance tomography to enhance sub-surface heterogeneity representation in HYDRUS 2D for simulating solute transport at the hillslope scale. 732 . . . . .	373
Online Fast Flow simulations for Discrete Fractured Media with Non-Standard Reduced Basis Method 157 . . . . .	374
Operator Splitting with Capillary Relaxation (OSCAR) 405 . . . . .	374
Optimal Fluid Stretching for Mixing-limited Reaction in Rough Fracture Flows 291 . . . . .	375
Optimal Irrigation control in Richards Equation Framework 600 . . . . .	376
Optimising site selection for hydrogen storage in porous rocks in the North Sea & Irish Sea 553 . . . . .	376
Optimizing gradient functional material for enhanced performance of solar-driven thermochemical fuel production 6 . . . . .	377
PORE-SCALE MODELLING IN SUPPORT OF SAFETY ASSESSMENT STUDIES FOR NUCLEAR WASTE REPOSITORIES IN FRACTURED ROCK 116 . . . . .	378
Parametrization of uncertainty for predictive modeling of subsurface flow problems 598 . . . . .	379
Particle Flow Through a Hydrophobic Nanopore 663 . . . . .	380
Particle transport and filtration in 2D and 3D porous media: coupling CFD and Deep Learning 585 . . . . .	380
Pattern formation controlled by friction and viscous forces in deformable granular media 549 . . . . .	381
Patterns in a reaction-diffusion double porosity system 406 . . . . .	382
Pedotransfer for infiltration estimation 416 . . . . .	383
Peltier Heats in Lithium-Ion Batteries 326 . . . . .	383
Permeability Decay Evaluation for a Nonlinear Oil flow through Porous Media in a Wellbore Near a Sealing Fault through Green's Functions (GF's) 277 . . . . .	384
Permeability Prediction via 3D Convolution Neural Networks 25 . . . . .	385
Perturbation Theory for Fluids under Confinement 475 . . . . .	386
Pesticide transport in unsaturated soils: from column tests to laboratory lysimeter. 476 . . . . .	386
Phase Transitions in Disordered Mesoporous Solids: Effect of Geometric Disorder 120 . . . . .	388
Phase behavior of a confined ionic discotic liquid crystal 182 . . . . .	388
Phase field fracture propagation with proppant transport and two phase flow 380 . . . . .	389
Phase-field modelling of bulk-surface PDEs and adhesive interfaces 573 . . . . .	390



Phase-wise conservative and physics-preserving algorithms for multi-phase flow in porous media 677 . . . . .	390
Physics Impact on Deep Neural Networks for Multiphase Flow in Porous Media 590 . . .	391
Plants control soil gas exchanges possibly via mucilage 648 . . . . .	392
Plug size pore network extraction with pore scale resolution 167 . . . . .	392
Poiseuillean viscous flows in menisci-bounded “bridges” and crevices of triangular pore channels: Blunt’s model revisited 397 . . . . .	393
Population balance models for particulate flows in porous media: breakage and shear-driven events 443 . . . . .	394
Pore Connectivity Analysis and Electrical Conductivity Model for Tight Sandstones 334 .	395
Pore Graded Anodic Transport Layers in PEM Electrolysers: A Pore Network Study 11 .	396
Pore Pressure Sensitivity-Permeability Decay Evaluation for Nonlinear Oil Flow in Porous Media through Green’s Functions (GF’s) 64 . . . . .	397
Pore Scale Visualization of CH <sub>4</sub> -CO <sub>2</sub> Mixed Hydrates Phase Transitions During Stepwise Depressurization 140 . . . . .	398
Pore network modeling of bubble ripening in porous media 442 . . . . .	398
Pore scale modelling of elastic properties of hydrate bearing sediment based on high resolution synchrotron x-ray computed tomography imaging 698 . . . . .	399
Pore scale two-phase simulation of viscous fingering of non-Newtonian fluids 143 . . . .	400
Pore-Scale Imaging of Tertiary Controlled-Salinity Waterflooding in a Heterogeneous Carbonate Rock at Reservoir Conditions 362 . . . . .	400
Pore-Scale Investigation of Nano-Enhanced Chemical Strategy for In-situ Crude Oil Contaminated Soils Remediation 707 . . . . .	401
Pore-Scale Simulation of Mucilage Drainage in the Rhizosphere 508 . . . . .	402
Pore-by-pore modeling, calibration, and prediction of two-phase flow in mixed-wet rocks 356 . . . . .	403
Pore-level observation of the transitional pore clogging by asphaltene deposition using micromodels 230 . . . . .	403
Pore-scale Investigation of the Capillary Pressure Effect on the Upward Migration of Hydrogen through Water-filled Porous Media 131 . . . . .	405
Pore-scale Mixing and the Evolution of Hydrodynamic Dispersion 733 . . . . .	406
Pore-scale analysis of gas injection in gas-condensate reservoirs 215 . . . . .	406
Pore-scale capillary heterogeneity in reservoir rocks and its influence on reservoir-scale flow 784 . . . . .	407

Pore-scale effects during the transition from capillary- to viscosity-dominated flow dynamics within microfluidic porous-like domains 567 . . . . .	408
Pore-scale hydro-mechanical modeling of gas transport in coal matrix 79 . . . . .	409
Pore-scale imaging of unsaturated solute transport to determine the influence of fluid distribution on solute spreading and mixing 364 . . . . .	409
Pore-scale modelling and sensitivity analyses of hydrogen-brine multiphase flow in geological porous media 104 . . . . .	410
Pore-scale observation and insight on how wettability impacts oil recovery and its dependence on rock structure 623 . . . . .	411
Pore-scale origin of flow-induced bio-aggregation 361 . . . . .	412
Pore-scale physics in imposed thermal gradient drying in porous media using Lattice Boltzmann Method 546 . . . . .	412
Pore-scale simulations of water droplet interaction with a hydrophobic wire screen for purpose of Water-Diesel separation 769 . . . . .	414
Pore-scale study to understand the influence of porosity on mass transport in Anodic Porous Transport Layer of PEM electrolyser using Lattice Boltzmann Method 510 . . . . .	414
Pore-throat structure and fractal characteristics of shale oil reservoirs in the Lucaogou Formation of Jimusaer Depression, China 10 . . . . .	415
Poromechanics in extremely large deformation: swelling and fracture 822 . . . . .	416
Porosity Dynamics through Carbonate-Reaction Kinetics in High-Temperature Aquifer Storage Applications 200 . . . . .	417
Porosity-permeability relationships for subflorescent salt crusts from evaporation of sand columns with varying initial salt concentration 204 . . . . .	418
Porous Media Flow as a Heat Sink in a Triple Layered Electromagnetic Heat Exchanger 743	419
Positive feedback effects in 2D creeping flow of viscoelastic fluids through porous media amplify preferential flow paths 342 . . . . .	420
Predicting the long-term thermal performance of EGS reservoirs from tracer tests using ensemble smoother with multiple data assimilation 520 . . . . .	420
Prediction of Flow and Reactive Transport using Physics-Informed Neural Networks 203	421
Process-dependent solute transport in porous media 141 . . . . .	422
Progress towards SAXS-based PEFC catalyst layer saturation determination 635 . . . . .	422
Promises, Challenges and Prospects of Deep Learning for Providing Insight into Multiphase Flow Through Porous Media 21 . . . . .	423
Quantification of non-linear multiphase flow in porous media for both water-wet and mixed-wet conditions 744 . . . . .	424

Quantification of uncertainty associated with the estimation of hydraulic parameters for saturated porous media 540 . . . . .	425
Quantifying Evolution of Mineral Reactive Surface Area and Pore Connectivity for Improved Prediction of Mineral Reaction Rates in Porous Media 746 . . . . .	425
Quantifying sulfate reduction rates of biofilm on shale fracture walls within a microfluidic reactor 652 . . . . .	426
Quantifying the corrosive influence of water and carbon dioxide on crack propagation in silica 376 . . . . .	427
Quick estimation of capillary pressure barrier of fractured caprocks. 664 . . . . .	427
RHEOLOGICAL RESPONSE OF FOAM FLOODING MODELS CONSIDERING EXPERIMENTAL UNCERTAINTIES 388 . . . . .	428
Random Emulation of Large-Scale Natural Pore Networks 14 . . . . .	429
Random Walks and Simplified Marching Cube for image-based simulations of heat or mass transfer in evolving porous media and applications to Ceramic-Matrix Composites 369 430	
Rapid spreading of complex fluids in porous substrates 804 . . . . .	430
Rayleigh-Taylor Instability in 2D and 3D Dispersive Porous Medium 576 . . . . .	431
Re-evaluation of the evolution and hysteresis of relative permeability in gas-brine systems: time to shift the paradigm? 318 . . . . .	432
Reaction-induced changes to structure and transmissivity of foamed wellbore cements 218 433	
Reactive CO <sub>2</sub> Density-Driven Flow in Aquifers 494 . . . . .	433
Reactive Imbibition of Acidic Fluids in Unconventional Shales: A New Experimental Approach to Pore-Scale Reactive Transport Modeling 82 . . . . .	434
Reactive Transport Modeling of Nanocapsules for Controlled Release of Cross-linking Agents for Conformance Control 740 . . . . .	435
Reconstructing contaminant release function in a sandbox experiment 685 . . . . .	436
Reconstruction of 3D shale digital rock based on generative adversarial network 616 . . . . .	437
Redox Flow Battery operation may be limited by “Hot Spots” observed in pore scale simulation of flow in carbon fibre felt electrodes 153 . . . . .	437
Reduced-dimensional models for flow in fractured porous media 125 . . . . .	438
Regimes of fluid-driven grain transport in a confined channel 473 . . . . .	439
Reinforcing and balancing feedback loops driven by dissolution and precipitation in reactive transport through porous media 787 . . . . .	440
Relative Permeability in Reactive Carbonate Rock 705 . . . . .	441
Relative contributions of permeability heterogeneity and viscosity contrast on scalar mixing 500 . . . . .	442

Remobilization of Colloids in Porous Media Under Unsaturated Condition in column-scale experiments 650 . . . . .	442
Representative elementary volume for Opalinus Clay from three-dimensional pore structure and transport analysis 611 . . . . .	443
Research on pore-scale hydrate permeability prediction based on machine learning 87 . .	444
Resolving flow path resistance in heterogeneous porous media as a graph-theory problem 777 . . . . .	444
Reversible Degradation of Diclofenac under Biotic, Denitrifying Redox Conditions: Geochemical Model and Uncertainty Quantification 437 . . . . .	445
Revisiting pedotransfer function databases by fitting dual porosity model and analyzing matrix and macro-pore properties 625 . . . . .	445
Rheology of a mixture of compressible and incompressible immiscible fluids in the capillary fiber bundle model 17 . . . . .	446
Rheology of two-phase flow in mixed-wet porous media: Dynamic network model and capillary fiber bundle results 18 . . . . .	447
Rigorous derivation of an effective model for reactive transport in evolving porous medium 207 . . . . .	448
Robust porous media flow control using Deep Reinforcement Learning 668 . . . . .	448
Root zone soil moisture estimation with Random Forest 419 . . . . .	449
Rotated Bounding Box Faster RCNN for Fracture Detection in X-Ray CT Image of Rocks 174 . . . . .	450
SIMULATION STUDY OF IN-SITU CONVERSION PROCESS IN LOW-MID MATURITY SHALE OIL RESERVOIR 89 . . . . .	451
Saturated Colloid transport experiments under unfavorable conditions in Dual-Porosity PDMS micro-models. 654 . . . . .	451
Scalable Multilevel Methods for Poroelasticity 735 . . . . .	452
Scaling and errors estimates of the effective Brinkman viscosity 722 . . . . .	453
Scaling of vertical mixing in two-species buoyancy-driven instabilities 679 . . . . .	453
Self-assembly of Comamonas denitrificans: formation of a living bacterial gel 726 . . . .	454
Self-sealing in wellbore cement under CGUS conditions by micro-CT, SEM, DM, and Raman 659 . . . . .	455
Semantic segmentation of microCT and FIB-SEM rock images using deep learning methods 455 . . . . .	455
Separation of colloidal particles in microchannels using diffusiophoresis 767 . . . . .	456
Shale microstructures: Experimental and fractal characterization 234 . . . . .	457

Shear Displacements of an Embedded Fracture Network using XFVM – a Sensitivity Analysis 467 . . . . .	457
Simple models of soil hydraulic properties in the complete moisture range: Testing the new PDI model system with a comprehensive experimental dataset 126 . . . . .	458
Simulating solute transport through saturated heterogenous medium using triple porosity non equilibrium model 713 . . . . .	459
Simulation of Thermochemical Heat Storage in the CaO/Ca(OH) <sub>2</sub> -System on the Micro-Scale 572 . . . . .	460
Simulation of blood flow in a whole mouse brain vasculature 671 . . . . .	461
Simulation of fractured porous media using partitioned black-box methods 186 . . . . .	461
Soil Moisture Data Fusion from Field Scale to Continental Scale 720 . . . . .	462
Solute Transport in Heterogeneous Soils from Different Land Management Practices 780	463
Solute transport during unstable infiltration into layered heterogeneous porous media 682	463
Soret effects in porous media 310 . . . . .	464
Spontaneous imbibition dynamics in yarns and knit stitches by fast X-ray tomography and free energy analysis 561 . . . . .	465
Stability and performance of emulsion in bulk-scale and pore-Scale 427 . . . . .	466
Stabilization of mine tailings using biological induced precipitation methods for wind erosion control 386 . . . . .	466
Statistical prediction of waterflooding performance by K-means clustering and empirical modeling 233 . . . . .	467
Steady-State Liquid Permeability Measurements in Ultra Tight Rock Samples 634 . . . . .	467
Stochastic 3D microstructure modeling for three-phase electrode materials with an emphasis on transport relevant characteristics 637 . . . . .	468
Stochastic homogenization of some porous media models 231 . . . . .	469
Strain evolution, faulting, and slow slip in Draupne shales 431 . . . . .	469
Strength and stability of fractured rocks 669 . . . . .	471
Study of convective drying of a mortar with a paste cover by NMR and MRI 191 . . . . .	472
Study of the Combined Effect of Reservoir Souring and Scale Formation in hydrocarbon reservoirs 781 . . . . .	472
Study of the impregnation process of electric engines' rotors with a reactive thermosetting resin: modeling and characterization of multi-physical coupling 358 . . . . .	474
Study of the mobility of zero-valent iron nanoparticles in porous media – Effect of grain size and composition 691 . . . . .	475

Study on Oil Recovery Effect and Mechanism of the Supercritical CO <sub>2</sub> Huff-n-Puff Process in Tight Cores with Nuclear Magnetic Resonance (NMR) 235 . . . . .	476
Study on poromechanical problems of hydrate sediment during phase transition process 304 . . . . .	477
Study on the Production Characteristics of Shale Oil using Machine Learning: Case Study of Jimsar Field 670 . . . . .	477
Study on the coupling mathematical model of gas-water two-phase seepage and wellbore pipe flow in fractured horizontal Wells in volcanic gas reservoirs 165 . . . . .	478
Study on the reuse of shut-down offshore platform 537 . . . . .	479
Studying viral aggregation in porous media 110 . . . . .	479
Sub-resolution feature size classification based on tunable X-ray dark-field imaging 545 . . . . .	480
Suction Cup System-Dependent Variable Boundary Condition: Transient Water Flow and Multi-Component Solute Transport 150 . . . . .	481
Surface Complexation Modeling on the Electrochemical Interactions of Low Salinity Wa- terflooding in Sandstone Reservoir 407 . . . . .	482
Surface-washing of contaminated porous substrates 752 . . . . .	482
Swelling beyond Flory 29 . . . . .	483
Synchrotron Microtomography Investigation of Nanoparticle Entrapment and Mobility in Porous Media 715 . . . . .	484
Targeted delivery of fertilizer in coarse textured soils using foam as carrier 325 . . . . .	485
The Alento hydrological observatory: An advanced open-air laboratory to evaluate the impact of anthropogenic disturbances on ecosystem services in a Mediterranean catch- ment. 527 . . . . .	486
The Chemical/Biological Remediation of Non-Aqueous Phase Liquids in Heterogeneous Porous Microfluidic Devices 201 . . . . .	487
The Effect of Surface Chemistry on Phase Behavior in Nanoporous Confinement: An Ex- perimental Study of iso-Butane Isotherms 759 . . . . .	488
The Effect of Surface roughness on the Equilibrium Contact Angle in a Mixed-Wet Medium 374 . . . . .	488
The Impact of Microscale Surface Roughness on Fluid Displacement Mechanisms and Resid- ual Saturations in Porous Media 94 . . . . .	489
The Importance of Microstructure in Redox Flow Batteries 164 . . . . .	490
The Influence of Motility on Bacterial Accumulation in a Microporous Channel 273 . . . . .	491
The Interplay of Spreading, Imbibition and Evaporation of Water Droplets on Nanoporous Surfaces 411 . . . . .	492
The Theory of Porous Media in Modelling Biological Tissues 821 . . . . .	493

The effect of the diffusion transport on CO <sub>2</sub> -water-rock reactions in CO <sub>2</sub> sequestration condition 345 . . . . .	493
The effect of tomographic imaging resolution on residual saturations during the drainage process 272 . . . . .	494
The effective boundary condition on a porous wall 30 . . . . .	495
The evolution of preferential flow paths during Enzymatically Induced Calcite Precipitation and its effect on the permeability 686 . . . . .	496
The effect of void structure on the permeability of fibrous networks 477 . . . . .	497
The impact of drought-induced root and root hair shrinkage on root-soil contact 559 . . . . .	497
The impact of pore scale complexity on fluid invasion patterns in heterogeneous rocks 68 . . . . .	498
The impact of roughness and wettability on imbibition in a fracture 379 . . . . .	499
The importance of accurate evapotranspiration forecast for crop irrigation: A global sensitivity analysis of two model case studies 311 . . . . .	500
The influence of surfactant flooding on oil displacement in Nano-Silica Pores 700 . . . . .	501
The morphology and surface-chemistry of gas-wetting nanoparticles and its effect on the liquid menisci in porous media 803 . . . . .	501
The relevance of simple probabilistic models for deposition, accumulation and transport of colloidal particles proved by real time, internal observations (MRI, confocal microscopy) 163 . . . . .	502
The role of collateral vessels in redistributing blood flow during stroke – combining in vivo data with blood flow simulations in semi-realistic networks using an inverse model 482 . . . . .	503
Theoretical analysis of poroelastic response of spherical indentation into a half space via step-displacement loading 776 . . . . .	504
Thermal fracturing and natural convection – a hidden source of geothermal activity in the earth’s crust? 632 . . . . .	505
Thermodynamic Stability of Bubble Population in Porous Media 541 . . . . .	506
Three-Dimensional Imaging of Density-Driven Convection in Porous Media Using X-ray CT Scanning 147 . . . . .	507
Threshold pressure for the capillary with irregular cross section 554 . . . . .	507
To biofilm or not to biofilm: Interplay between chemotactic dispersal and biofilm formation in bacterial communities 290 . . . . .	508
Toolchain from the creation of the mesh to the CFD simulations 58 . . . . .	509
Tortuosity and permeability of random porous medium using deep learning 159 . . . . .	510
Towards Geologic CO <sub>2</sub> Sequestration at Scale: A Review of Geomechanical Impacts, Induced Seismicity Concerns, and Mitigation Measure 71 . . . . .	511

Towards HPC simulations of Billion-cell Reservoirs by Multiscale Mixed Methods 795 . . .	511
Towards Unified Pore-Scale Imaging and Modelling: Comparison of the Generalized Network Model with Direct Numerical Simulation 487 . . . . .	512
Towards bottom-up design of porous electrode microstructures - coupling genetic algorithms with pore network modeling of redox flow battery electrodes 566 . . . . .	513
Towards scalable multi-scale open-source solvers for ionic transport and electrochemistry 206 . . . . .	514
Transdisciplinary Soil Hydrology 95 . . . . .	515
Transient ground water level simulation scale with pre-calculated time-varying recharge values 385 . . . . .	516
Transport analysis in deformable porous media through integral transforms 499 . . . . .	517
Transport of chemotactic bacteria in porous media with residual sources of chemical pollutants 808 . . . . .	517
Transport properties modelled on multiscale porous media images 465 . . . . .	518
Transport-Related Consequences of Geochemical Interactions between Shale, Formation Brine, and Reactive Fluid 760 . . . . .	519
Two-grid coupled multiphase flow and geomechanics: A computational framework to monitor surface deformation along with fault slip due to pore pressure perturbations 463 . . . . .	520
Two-scale poromechanical model incorporating adsorption effects of a fluid mixture in arbitrary geometrical nanopores 359 . . . . .	520
Uncertainty Quantification of Relative Permeability Measurements by Inverse Modelling 23 . . . . .	521
Uncertainty-aware Validation Benchmarks for Coupling Free Flow and Porous-Medium Flow 454 . . . . .	522
Under pressure: Hydrogel swelling in a granular medium 773 . . . . .	523
Underground Hydrogen Storage: a multiscale experimental-numerical study 807 . . . . .	524
Understanding Electrolyte Infilling for Lithium Ion Batteries 470 . . . . .	524
Understanding dynamic pore-scale interactions for underground hydrogen storage through high resolution 3D X-ray imaging 330 . . . . .	525
Understanding the combined effect of structural and wettability heterogeneity on two-phase flow in porous media 438 . . . . .	526
Understanding the influence of pore-scale rock heterogeneity in CO <sub>2</sub> geo-sequestration 626 . . . . .	528
Understanding the mechanisms of the brain's waterscape 796 . . . . .	528
Unified multiphysics framework for assessment of CO <sub>2</sub> storage in heterogeneous saline aquifers 254 . . . . .	529



Unsaturated Flow Effects on Solute Transport in Soils 239 . . . . .	530
Unsaturated hydraulic properties in a nearly saturated medium 172 . . . . .	530
Unsaturated porous media freezing: numerical modeling and validation based on experimental data 216 . . . . .	531
Upscaling Inertia Effects on Mixing and Reaction at Channel Intersections from Flow Topology 422 . . . . .	532
Upscaling between an agent-based model (smoothed particle approach) and a continuum-based model for wound contractions 142 . . . . .	533
Upscaling of a Cahn–Hilliard Navier–Stokes Model including Precipitation in a Thin Strip 579 . . . . .	534
Upscaling of two-phase flows in porous media 219 . . . . .	534
Upscaling reactive flow and transport in evolving porous media 100 . . . . .	535
Use of DNA tracers for determining aquifer hydraulic properties in a 3-dimensional laboratory sand tank 558 . . . . .	536
Use of infrared nano-spectroscopy to study the existence and thickness of the wetting film in oil-wet carbonates 750 . . . . .	536
Use of porous algal biochar in water treatment in the state of Ceará in Brazil 563 . . . . .	537
Use of topological principles to determine wettability from pore-scale images 511 . . . . .	538
Using PIV and 3D printing to investigate fluid flow and solute transport in fractured porous media. 177 . . . . .	539
Using colloidal deposition to mobilize immiscible fluids from porous media 286 . . . . .	540
Validation and calibration of interface conditions for Stokes-Darcy problems 458 . . . . .	541
Variations in Airflow Field and Soil Grain-Size of Simulated Shrubs with Different Spatial Configurations based on Wind Tunnel Experiments 417 . . . . .	541
Viscous Fingering in Miscible Displacements in Porous Media with Dead-End Pores 601 . . . . .	542
Visualization Research of Clay Mineral Migration in Low Salinity Water Flooding Based on 2.5D Microfluidic Model 327 . . . . .	543
Visualization and segmentation of micro-cracks based on X-ray computed tomography imaging 357 . . . . .	544
Visualization of optically opaque flow systems through lab-based, dynamic X-ray micro-CT 472 . . . . .	545
Visualizing imbibition in thin porous media with high-speed NMR 197 . . . . .	546
Water infiltration to sandstone outcrops at the soil-rock interface 413 . . . . .	547
Water transport in soft nanoporous materials: Impact of mechanical deformation on collective dynamics, interfacial slippage and permeance 320 . . . . .	548

Wettability behavior of preserved core material compared to dry stored core plugs during a low salinity water core-flooding investigation 736 . . . . .	548
Wettability effects on multiphase displacements in heterogeneous porous media 620 . . .	549
Wetting, Imbibition and Switchable Elastocapillarity in Nanoporous Media 264 . . . . .	550
Investigation of water freezing in gas diffusion layer of PEMFC using lattice Boltzmann method 258 . . . . .	551
the impacts of pore-scale two-phase flow on mineral reaction rate 587 . . . . .	552
'Cocktail effects' of co-existing hydrocarbon on heavy metal remediation 811 . . . . .	552

**Invited & Keynote Speakers / 814****3D Magnetic Resonance Imaging Studies of Porous Media: From Operando Catalysis to Fluid Transport in Rock Cores****Author:** Lynn Gladden<sup>1</sup><sup>1</sup> *University of Cambridge***Corresponding Author:** lfg1@cam.ac.uk

Magnetic resonance techniques are well-established in application to studying structure-transport relationships in porous media. This presentation will focus around studies of two porous media systems: heterogeneous catalysis and fluid transport in rock cores. A range of magnetic resonance techniques are employed. The basic principles of these methods will be explained. In particular, the contribution made by combining undersampling and compressed sensing image reconstruction techniques with standard magnetic resonance acquisitions will be summarized.

**Operando Catalysis:** The main focus of our work is to understand catalytic behavior at real operating conditions in a representative process environment, and hence gain insight into catalyst design and optimal process operating conditions. Reactions of interest to date have been ethene oligomerization and Fischer-Tropsch synthesis. We can now measure molecular diffusion within the pores of catalysts while they are operating, and track gas and liquid phase composition as a function of time-on-stream. By spatially mapping diffusion measurements it becomes possible to see how molecular processes in the catalyst pores vary along the length of a tubular reactor.

**Fluid Transport in Rock Cores:** Understanding how fluids flow through porous media has been a topic of long-standing research interest with regard to optimizing hydrocarbon recovery processes. More recently, research interest is moving to even more challenging problems such as carbon sequestration and hydrogen storage. We will show how three-dimensional (3D) images of fluid flow velocity within the porous structure of rocks can be measured at an isotropic spatial resolution of 35 microns. These maps can then be co-registered with magnetic resonance images of the pore structure or with higher resolution X-ray microtomography datasets to enable us to explore structure-flow correlations within the rocks. These data are of interest in their own right and, of course, provide invaluable data with which to validate and hence develop numerical simulation codes.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:****Acceptance of Terms and Conditions:**Click here to agree **Newsletter:**I do not want to receive the InterPore newsletter **Student Poster Award:****Poster + / 84****3D adaptive modelling of transient multiphase flow experiments using the MOOSE framework****Author:** Samuel Jackson<sup>1</sup>**Co-authors:** Chris Green<sup>1</sup> ; Mojtaba Seyyedi<sup>1</sup> ; Michael Clennell<sup>1</sup><sup>1</sup> *CSIRO***Corresponding Authors:** chris.green@csiro.au, ben.clennell@csiro.au, mojtaba.seyyedi@csiro.au, samuel.jackson@csiro.au

Fluid-fluid displacements with adverse viscosity ratios are prone to instability, and their interaction with underlying heterogeneity in a porous medium can cause a variety of fingering structures to

emerge. The transient dynamics of these processes are both hard to capture experimentally, and difficult to model numerically, leading to conflicting studies with differing mechanisms for their origins [1,2].

In this work, we develop a novel adaptive mesh modelling approach to rigorously and transparently model continuum-scale transient multiphase flow in heterogeneous media. We use the MOOSE framework ([www.mooseframework.org](http://www.mooseframework.org)) - an open-source multiphysics simulation platform [3]. We use a finite-volume approach with automatic differentiation and adaptive octree meshes, which evolve with the moving front. Petrophysical parameters are pre-computed for multiple levels of the octree structure, allowing efficient and physically accurate refinement of the computational grid as the simulation progresses. The approach allows the simulation of large flow domains with high precision, mesh-independent resolution of unstable fingering structures and moving front interactions with truly heterogeneous regions of a porous media.

We use the simulation approach to model several metre-scale experiments performed in Bentheimer and Boise rock cores. In the experiments, nitrogen-brine flow was imaged dynamically with a novel Medical-CT setup, allowing plume tracking and 3D resolution of fingering structures at mm-scale over the metre-long cylindrical cores. We compare the transient dynamics of the front with those directly from our simulations at a variety of scales, leaving no ambiguity in the efficacy of the modelling approach. We directly visualise the competition between fluid-fluid and fluid-structure based instability, and the onset of fingering at the continuum scale.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

[1] Berg, S & Ott, H (2012). Stability of CO<sub>2</sub>-brine immiscible displacement. *International Journal of Greenhouse Gas Control*, 11, 188-203.

[2] Sorbie, K.S., Al Ghafri, A.Y., Skauge, A. et al. (2020). On the Modelling of Immiscible Viscous Fingering in Two-Phase Flow in Porous Media. *Transport in Porous Media* 135, 331–359.

[3] Wilkins, A., Green, C. P., & Ennis-King, J. (2020). PorousFlow: a multiphysics simulation code for coupled problems in porous media. *Journal of Open Source Software*, 5(55), 2176. **Acceptance of Terms and Conditions:**

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**Student Poster Award:**

Poster + / 628

## 3D-1D coupling on non-conforming meshes via an optimization based three-field domain decomposition approach

**Authors:** Stefano Berrone<sup>1</sup> ; Denise Grappein<sup>2</sup> ; Stefano Scialò<sup>2</sup>

<sup>1</sup> *Politecnico di Torino, Italy*

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A new numerical approach is proposed for the simulation of coupled three-dimensional and one-dimensional elliptic equations (3D-1D coupling). Possible applications are the interaction of a capillary network with the surrounding tissue, of tree roots with the soil, or of a system of wells with a reservoir in geological applications. In all of these cases, in which nearly 1D fractures are embedded in a much wider porous matrix, the generation of a 3D mesh inside the small inclusions can become extremely expensive, as well as the resolution of the resulting discrete problem. For these reasons we developed [1] a novel framework for 3D-1D coupling based on a well posed mathematical formulation and with a high robustness and flexibility in handling geometrical complexities. This is achieved by means of a three-field domain decomposition [2] to split the reduced 1D problems from the bulk 3D problem, and then resorting to the minimization of a properly designed functional to

impose matching conditions at the interfaces, following an approach similar to the one used for handling discrete fracture networks in [3]. Thanks to the structure of the functional, the method allows to use completely independent meshes on the various subdomains and on the interfaces.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

- [1] S. Berrone, D. Grappein, S. Scialò, “3D-1D coupling on non-conforming meshes via three-field optimization based domain decomposition”. arXiv:2102.06601
- [2] F. Brezzi, L. Marini, “A three-field domain decomposition method,” Contemporary Mathematics 157 (1994)
- [3] S. Berrone, D. Grappein, S. Pieraccini, S. Scialò, “A three-field based optimization formulation for flow simulations in networks of fractures on non-conforming meshes”, accepted for publication on SIAM J. Sci. Comput. (2019). arXiv:1912.09744 **Acceptance of Terms and Conditions:**

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Poster + / 491

## 4D Investigation of groundwater remediation using nanotechnology-a synchrotron-based X-ray micro-tomography study

**Authors:** Tannaz Pak<sup>1</sup> ; Luiz Fernando de Lima Luz Junior<sup>2</sup> ; Tiziana Tosco<sup>3</sup> ; Paola Rodrigues Rangel Rosa<sup>4</sup> ; Gabriel Schubert Ruiz Costa<sup>4</sup> ; Nathaly Lopes Archilha<sup>4</sup>

<sup>1</sup> Teesside University

<sup>2</sup> Federal University of Paraná

<sup>3</sup> Politecnico di Torino

<sup>4</sup> Brazilian Synchrotron Light Laboratory (LNLS) - Brazilian Centre for Research in Energy and Materials (CNPEM)

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Reactive transport in porous media is a dynamic field of research with open questions particularly at pore-scale. Despite our detailed understanding of non-reactive multiphase flow in porous media, across scales, little is known about the pore-scale dynamics of processes involving chemical reactions alongside fluid flow in porous media. Reactive flow plays a key role in a range of application including groundwater remediation, CO<sub>2</sub> sequestration, metal recovery, and heavy oil recovery. In these processes a chemical reaction is engineered to impact the structure/properties of the host porous medium or the arrangement of fluids it confines. In this contribution we study the classic problem of groundwater contamination with chlorinated solvents but from a pore-scale perspective. Chlorinated solvents are known as a persistent family of aquifer contaminants which, over the past decades, have caused serious health problems (e.g. kidney and liver damage) and some are considered as carcinogenic. Being denser than water, when a leakage occurs at the surface these contaminants sink into the groundwater system and create a source of contamination in form of trapped DNAPLs (i.e. dense non-aqueous phase liquids). The scale of the problem posed by these contaminants is globally significant due to their wide industrial use since the beginning of 20th century e.g. in metal processing plants and dry cleaning.

In this work we performed a synchrotron-based micro-tomography imaging experiment to study the dynamics of the reactive transport process during application of nanoremediation<sup>1</sup>. Nanoremediation is a new technology that injects aqueous suspensions of zero valent iron nanoparticles (nZVI) into contaminant bearing subsurface sediments. These nanoparticles are highly reactive and excellent electron donors ( $\text{Fe}^0 \rightarrow \text{Fe}^{2+} + 2\text{e}^-$ ). Chlorinated solvents accept those electrons and release their chlorine atoms in form of ions. Example reaction: ( $\text{C}_2\text{H}_2\text{Cl}_2 + \text{Fe}^0 + 2\text{H}^+ \rightarrow \text{C}_2\text{H}_4 + 2\text{Cl}^- + \text{Fe}^{2+}$ ). While nanoremediation concept is proven to be successful at laboratory, pilot, and field scales, the existing practice is far from optimised. A contributing factor to this is the lack of understanding around pore-scale mechanisms that control the nanoremediation process.

Our 4D (time-resolved, 3D) experiment comprised of fluid injections in a column (packed with glass beads) and simultaneous 3D imaging using X-ray micro-CT technique. The study was conducted at the Brazilian synchrotron. For the first time, we captured the evolution of the DNAPL phase structure/distribution, in 3D, during the nanoremediation process. Our data show that a gas phase is released during nanoremediation which remobilises the trapped DNAPL phase, facilitating its complete removal in subsequent soil flushing processes. Our findings also show the evolved gas reduces the relative permeability of the contaminated water phase from 60% to less than 1%. This suggests that the gas evolution provides a temporary control on the contamination plume propagation. This favourable outcome is caused by pore-scale blockage of water flow-pathways by the released gas. In field applications of nanoremediation (or similar in-situ remediation technologies) gas formation is considered as a sign of effectiveness of the process. This study provides a quantitative evidence on how this gas release can impact the contamination removal and limit its propagation.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

Pak, T. et al. Pore-scale investigation of the use of reactive nanoparticles for in situ remediation of contaminated groundwater source. *Proc. Natl. Acad. Sci.* 117, 201918683 (2020). **Acceptance of Terms and Conditions:**

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**Student Poster Award:**

**MS10 / 486**

## **4D $\mu$ CT reconstruction with improved time resolution for imaging fluid flow in porous media**

**Authors:** Wannas Goethals<sup>1</sup> ; Jan Aelterman<sup>2</sup> ; Tom Bultreys<sup>2</sup> ; Matthieu Boone<sup>1</sup>

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<sup>2</sup> Ghent University

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Computed micro-tomography ( $\mu$ CT) is a valuable tool to study transport phenomena in the 3D pore network of geomaterials. Recent advances, mainly at synchrotron beam lines but also using lab scanners, have made it possible to perform time-resolved  $\mu$ CT, imaging changes in the sample over time, with time resolutions on the order of seconds. In such cases, a 4D reconstruction is computed from a set of radiographs acquired during multiple rotations of the sample relative to the X-ray source and detector. Typically, a single 3D volume is computed to represent the time period associated with its set of radiographs, often inaccurately thought of as a single point in time, a time step. Therefore, during the acquisition of a single time step, dynamic changes in the sample (e.g. fluid occupancy) give rise to motion artifacts, which deteriorate the final image. A standard cone beam  $\mu$ CT reconstruction of a sample during capillary-dominated drainage (figure A) illustrates how sudden pore-scale fluid displacements disturb the results in the neighborhood of these pores. This may affect further analysis, e.g. the measurement of contact angles in two-phase flow experiments. To reduce these motion artefacts, it is key to keep the acquisition time as short as possible while still achieving a sufficiently high image quality.

To increase the time resolution of a typical  $\mu$ CT measurement several fold, the reconstruction approach presented here drastically limits the angular range of each time step. This shortens the considered time period, lessening the impact of motion artifacts. To compensate for the associated limited angle artefacts (illustrated in figure B), we propose to incorporate temporal total variation (TV) minimization into an iterative reconstruction technique (figure C). This temporal regularization effectively restores the spatial structure, while still resolving salient changes in the sample over time.

To validate the method, a synthetic dynamic 2D  $\mu$ CT dataset of a drainage experiment was created. Reconstructions were made with various angular window sizes (ranging from  $12^\circ$  to  $200^\circ$ ), representing a *potential* increase of a factor 16.7 in the time resolution. The temporal attenuation curve of each pore was compared for the proposed technique and for a standard reconstruction. The improvements in time resolution of the  $\mu$ CT reconstructions with temporal TV minimization were quantified and found to be significantly improved. Application of the method to real measurement data suggests its suitability and usefulness towards imaging dynamic processes in porous materials.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Berg, S., Ott, H., Klapp, S. a, Schwing, A., Neiteler, R., Brussee, N., et al. (2013). Real-time 3D imaging of Haines jumps in porous media flow. *Proceedings of the National Academy of Sciences*, 110(10), 3755–3759. <https://doi.org/10.1073/pnas.1221373110>

Bultreys, T., Boone, M. A., Boone, M. N., De Schryver, T., Masschaele, B., Van Hoorebeke, L., & Cnudde, V. (2016). Fast laboratory-based micro-computed tomography for pore-scale research: Illustrative experiments and perspectives on the future. *Advances in Water Resources*, 95, 341–351. <https://doi.org/10.1016/j.advwatres.2015.05.012>

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**Poster + / 642**

## A (dual) network model for heat transfer in porous media

**Authors:** Timo Koch<sup>None</sup> ; Kilian Weishaupt<sup>1</sup> ; Johannes Müller<sup>None</sup> ; Bernhard Weigand<sup>1</sup> ; Rainer Helmig<sup>1</sup>

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We present a new concept for modelling single-phase flow and energy transport in porous media including conditions under which local thermal equilibrium cannot be assumed. A dual network model is introduced based on a recently developed algorithm to represent both the pore space and the solid grain matrix in a porous medium by interconnected networks.

Heat and mass transfer are considered simultaneously, allowing to naturally model scenarios with heterogeneous temperature distributions in both void space and solid matrix. We suggest a discretisation of mass, momentum, and energy balance equations using a dual network representation.

The new approach is compared with 3D conjugate heat transfer simulations for both conduction- and convection-dominated scenarios.

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**MS7 / 381**

## A 6M Digital Twin for Reservoirs

**Authors:** tao zhang<sup>1</sup> ; Shuyu Sun<sup>2</sup>

<sup>1</sup> King Abdullah University of Science and Technology

<sup>2</sup> King Abdullah University of Science and Technology (KAUST)

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Modeling and simulation of flow, transport and geomechanics in the subsurface porous media is an effective approach to help make decisions associated with the management of subsurface oil and gas reservoirs, as well as in other wide application areas including groundwater contamination and carbon sequestration. Accurate modeling and efficient, robust simulation have always been the main purposes of reservoir researches, and a 6M digital twin (multi-scale, multi-domain, multi-physics and multi-numeric numerical modeling and simulation of multi-component and multi-phase fluid flow in porous media) is designed, equipped with the following six pronounced features, to better digitally model and simulate the engineering processes and procedures in physical reality and further control and optimize such processes and procedures: 1. Efficient and reliable flash calculation; 2. Advanced phase interface modeling; 3. Fully conservative bound-preserving Darcys scale flow simulation; 4. Reactive flow and transport in porous media; 5. Molecular simulation of microscopic mechanisms; 6. High-performance computation based on fully-implicit and bound-preserving algorithms.

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MS13 / 382

## A DFT study on the effect of strain on the adsorption of gas in tight gas carbonates

**Author:** Elkhansa Elbasher<sup>1</sup>

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Tight unconventional reservoirs are characterized by structural complexation and physical properties that influence the ability to recover and estimate the amount of gas in the rock. One of the physical factors is the change of the strain which may affect the gas interaction with the rocks' surface. To study the effect of strain on the gas-surface interaction, density functional theory (DFT) calculations are conducted to find the adsorption energy of the natural gas' components on the tight-gas carbonated reservoirs. Calcite (104) represents the majority of the calcium carbonate reservoirs; thus, it is selected in this work to represent the tight reservoirs. The gases considered in the study are CH<sub>4</sub>, CO<sub>2</sub>, C<sub>2</sub>H<sub>6</sub>, and N<sub>2</sub>, and they all show a physiochemical interaction with the surface for all the considered strain values (-3% to 3%), with CO<sub>2</sub> showing the highest adsorption affinity. Along with the weak interaction, there is no specific trend for the change of CH<sub>4</sub> adsorption with the strain effect. In contrast, the change in adsorption of CO<sub>2</sub> and C<sub>2</sub>H<sub>6</sub> showed more pronounced alteration with strain compared to other gases. For instance, by applying tensile strain, a 25% increase in CO<sub>2</sub> adsorption energy is obtained depending on the concentration of the gas molecules. The estimation of ultimate recovery (EUR) could be determined from the obtained results by computing the effects



of the geomechanical factors on the adsorption of the gas on the surface of the carbonaceous tight gas reservoirs.

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MS17 / 232

## A Darcy scale coupled fluid-thermal framework to model radionuclide transport from a deep disposal borehole

**Authors:** Kaveh Sookhak Lari<sup>1</sup> ; Dirk Mallants<sup>1</sup>

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Waste packages for disposal of radioactive waste originating from reprocessing of spent nuclear fuel typically include a stainless steel canister inside which the waste is immobilised in a (borosilicate) glass matrix. A potential disposal pathway for such wastes is in conventional mined geological disposal facilities (GDF) [1] or in deep boreholes [2]. In the latter concept, the packages are stacked in a disposal zone at a depth of several kilometres [3]. However, deep borehole disposal is still in its infancy requiring considerable Research, Development and Demonstration (RD&D) to bring the science to a similar level as for GDFs [4].

It is estimated that the total global inventory of radioactivity confined within (borosilicate) glass from reprocessing is on the order of  $10^{20}$  Bq, with an approximate weight of 15,000 metric tonnes [5, 6]. The half-life of some of the radionuclides in nuclear waste is from the order of  $10^5 - 10^9$  y (e.g.  $^{135}\text{Cs}$ ,  $^{79}\text{Se}$ ,  $^{238}\text{U}$ , etc) [6]. This waste will generate heat for several hundred years [7, 8]. Any disposal container should have a lifetime long enough to survive (i.e. no breach therefore zero release) the heat-production period.

For clay sediments, a porous medium-type pore network is the path through which transport occurs [9]. For crystalline rocks on the other hand, transport is typically through a fracture network with concomitant matrix diffusion [1]. The nonlinear interaction between different transport phenomena and the very long time scales of the processes involved, necessitates modelling as the most realistic tool to assess the risks to humans and the environment [10]. Given the much greater disposal depth of a deep borehole concept compared to conventional GDFs, and the heat-generating feature of the disposed waste, temperature evolution and its potential impact on radionuclide migration has to be accounted for in post-closure safety assessments.

For conventional GDFs, several studies have been conducted to model the thermal, hydraulic and mechanical interactions within the near field of the disposal environment [11]. The majority of these post-closure safety assessments consider isothermal transport of dissolved radionuclides, using simulation codes such as FRAC and PORFLOW [10, 12]. Some studies have also used TOUGH or TOUGHREACT to couple other transport phenomena [13]. However, few modelling studies exist for deep borehole disposal which include a proper linkage between the natural hydrostatic and temperature profiles to heat and solute mass transport at the Darcy scale [14, 15].

Here we present a coupled heat and solute mass transport modelling framework, subjected to depth-dependent temperature, pressure and viscosity profiles - assuming an instantaneous release of all radionuclides. This is a very conservative assumption but is consistent with typical "what if?" scenarios undertaken in post-closure safety assessments [16]. The TOUGHREACT code [17, 18] was used in an axi-symmetrical domain with a total depth of 3200 m. Several scenarios of heat-generation were investigated to test if the additional heat produced by the waste containers affects radionuclide migration, e.g. by generating convection-driven mass transport. Results show that the heat generation does not significantly affect the extent of the solute mass plume.

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MS9 / 619

## A Dynamic Hybrid Multiscale Model for Simulating Flow and Mixing-Controlled Reactions in Porous Media

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Mixing-controlled reactions govern various systems, and play a central role in many industrial applications (e.g., CO<sub>2</sub> sequestration and microbially-induced calcite precipitation). However, at-scale models are limited in simulating such processes with high fidelity and computational efficiency, especially in describing those reactively “hot spots” that often occur at fundamental scales but having significant effects on larger-scale system behaviors. In this study, we present a domain-decomposition based hybrid multiscale model combined with adaptive criteria that can dynamically determine pore-scale subdomains where/when needed and simulate pore-scale and Darcy-scale processes concurrently, namely the dynamic hybrid multiscale model (dHMM). Pore- and Darcy-scale multiple-relaxation-time lattice Boltzmann models (MRT-LBMs) are loosely-coupled in an iterative way via proper boundary conditions through a multiscale universal interface. To facilitate pore-scale subdomains, a dynamic threshold calculated based on real-time concentration distribution is utilized. Simulated results are first validated by comparing with analytical solutions. The dHMM is then applied to simulate mixing-controlled bimolecular reactions in both homogeneous and heterogeneous porous media. Results are cross-compared with data computed from our previously-developed HMM and at-scale models. We demonstrate that the dHMM serves as a powerful tool for numerical up-scaling and studying the effects of small-scale processes to large-scale systems.

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MS3 / 687

## A Flow Discretization for Conforming Discrete Fracture Matrix Models with Upscaling of Microscale Fractures

**Authors:** Eirik Keilegavlen<sup>1</sup>; Alessio Fumagalli<sup>2</sup><sup>1</sup> *University of Bergen*<sup>2</sup> *Politecnico di Milano***Corresponding Authors:** eirik.keilegavlen@uib.no, alessio.fumagalli@polimi.it

Natural occurring fractures can dominate fluid flow in subsurface rock and thus be crucial for engineering operations such as energy recovery and waste disposal. The fractures occur on multiple length scale with no scale separation, forming a challenge for their incorporation into mathematical models for fluid flow [1], as well as for discretizations.

Among the several classes of conceptual models for representing fractures [2], our interest is in the so-called Discrete Fracture Matrix (DFM) models. In DFM models, fractures that are deemed important (here termed macroscale fractures) are explicitly represented allowing for detailed representation of dynamics in these fractures, while the remaining (herein microscale) fractures are upscaled into equivalent continuum properties. We further consider DFM models where the fractures are represented as lower-dimensional objects and where the computational mesh conforms to these objects. This approach allows for high modeling and discretization of complex multiphysics processes [3], to the price of relatively high computational cost due to the high cell count needed to resolve the fractures.

The high computational cost makes the task of fracture upscaling critical for the feasibility of DFM methods with conforming grids. While discretization methods for this class of models have received much attention over the last decade, techniques for upscaling those fractures that are not explicitly represented have not been much studied.

In this work, we present a conforming DFM approach for the flow problem with a discretization that is tailored for upscaling of microscale fractures. The computational mesh is constructed to conform with the macroscale fractures. Inspired by the Multiscale Finite Volume [4] method, the basis functions for discretization on this macro mesh are constructed by solving local (to small patches of macro cells) problems where the microscale fractures are explicitly represented. This approach allows us to represent complex fracture networks at a reasonable computational cost. Moreover, re-labeling of fractures between macro and micro is relatively straightforward, allowing for the study of the interplay between computational cost and errors due to upscaling and macro- and micro discretization. The implementation is open source [5] and is based on a standard workflow for meshing and discretization of conforming DFM models [6].

We present numerical examples for complex fracture networks in 2d and 3d, with emphasis on accuracy, convergence and robustness of the numerical methods. We also illustrate the impact of upscaling versus explicit representation on fracture networks where there is no separation of fracture length scales.

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MS7 / 363

## **A Graphical Representation of Membrane Filtration with Adsorption**

**Authors:** Binan Gu<sup>1</sup> ; Linda Cummings<sup>1</sup> ; Lou Kondic<sup>1</sup>

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We study the performance of a membrane filter represented by a pore network based on two criteria: 1) total volumetric throughput and 2) accumulated foulant concentration. We first formulate the governing equations of fluid flow on a general network, and we model adsorptive fouling by imposing an advection equation on each pore (edge) and imposing conservation of fluid and foulant volumetric flow rate at each pore junction (vertex), which yields a system of partial differential equations. We study the influence of three geometric network parameters on filter performance: 1) average number of neighbors of each vertex; 2) initial total void volume of the pore network; and 3) tortuosity of the network. We find that total volumetric throughput has a stronger dependence on the initial void volume than on average number of neighbors. Tortuosity turns out to be a universal parameter, leading to almost perfect collapse of all results for a variety of different network architectures. In particular, the accumulated foulant concentration shows an exponential decay as tortuosity increases.

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MS6-B / 61

## A Laboratory Study of Foam Coarsening in Model Fractures

**Author:** Kai Li<sup>1</sup>

**Co-authors:** Mohammadamin Sharifnik<sup>2</sup>; Karl-Heinz Wolf<sup>1</sup>; William Rossen<sup>1</sup>

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Foam is composed of gas bubbles separated by continuous liquid films. The films, called lamellae, are stabilized by surfactants. Foam has many applications in underground resources, such as acid stimulation (Thompson and Gdanski 1993), aquifer remediation (Hirasaki et al. 1997) and enhanced oil recovery (Kovscek and Radke 1994; Rossen 1996). In enhanced oil recovery, foam injection can improve sweep efficiency by reducing the mobility of gas. To achieve an optimized mobility control, the stability of foam must be maintained while it propagates deep into the reservoir. At the pore scale, the coalescence of foam can take place due to different mechanisms including capillary coalescence and diffusive coarsening. Coarsening behavior has been well studied in bulk foam (Weaire and Glazier, 1993; Weaire and Hutzler, 1999). However, it is less understood in porous media.

In this study, we have built two 1-meter-long model fractures analogous to microfluidic porous media, and investigate the effects of coarsening on static foams in the models. The model fractures are made of glass plates. Direct observation and analysis of the foam structure inside the fractures are facilitated using a high-speed camera. Each model fracture has one flat wall and one rough wall. The gap between the two walls represents the aperture of the fracture. The distribution of aperture can be represented as a 2D map of pores and throats. We use two model fractures with different roughness distributions. One model has a roughness in a regular pattern with a hydraulic aperture of 46  $\mu\text{m}$ . The other one has an irregular pattern with a hydraulic aperture of 80  $\mu\text{m}$ .

Prior to coarsening, foam is pre-generated, and then injected into the fractures. After foam flow reaches steady-state, the injection and production valves are closed. Once foam stops flowing, as the residual pressure gradient dissipates, the coarsening process commences.

In this study, we have observed that the foam coarsens due to gas diffusion in both model fractures. Due to coarsening, bubble numbers decrease and bubble size increases. The time scale of coarsening in our models is much larger than what has been reported elsewhere (Marchalot et al., 2008; Jones et al., 2018). In the regular model, coarsening stops after 2 hours. At the end of coarsening, all lamellae have zero curvature and rest at pore throats. Bubbles attain the same size as pores and almost all

the liquid accumulates in plateau borders at throats. Compared to the regular model, the coarsening process is slower in the irregular model. Bubbles coarsening slows down to a barely-measurable diffusion rate after 7 hours. However, small bubbles exist and the average bubble size increases even after 24 hours of coarsening. A possible explanation is that, for these small bubbles, the lamella area available through which gas can diffuse to a neighbouring larger bubble is greatly reduced. In both models, the capillary pressure increases to 1.3 kPa, which is too low to cause lamellae to break.

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MS7 / 738

## **A Maximum Principle Preserving Finite Element Method with Mass Conservation Property for Solving Two-Phase Flow in Heterogeneous Porous Media**

**Author:** Mohammad Sarraf Joshaghani<sup>1</sup>

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We present a first-order finite element method with mass-lumping and flux upwinding, to solve the immiscible two-phase incompressible flow problem in porous media. The primary unknowns are the wetting phase pressure and saturation. Recently, the theoretical convergence analysis of the method was derived in [1]. Here, we propose a comprehensive computational methodology and extend the scheme to heterogeneous porous media, which makes the method appealing to reservoir simulators. Numerical examples of quarter-five spot problems in two and three dimensions, confirm that the method is accurate, and robust, even in the case of realistic discontinuous highly varying permeability. We also show that the proposed method is locally mass-conservative and the resulting solutions satisfy the maximum principle. The method is mesh-independent and does not require penalization or any external bound-preserving mechanism.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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MS10 / 655

## A Novel Technique of Image Analysis on Foam in Fractures

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In enhanced oil recovery, gas injection often suffers from poor sweep efficiency due to conformance problems, such as gravity override, viscous fingering and channelling. Foam, composed of gas bubbles separated by continuous liquid films (lamellae), can effectively mitigate these problems. During foam flooding, the mobility of gas is reduced by a factor of hundreds or even more (Tang and Kovscek, 2006). As a result, the displacement front is more stable, and more gas is diverted to unswept zones, hence improving the sweep and recovery.

The ability of gas mobility reduction of foam is highly dependent on its texture. It has been found that foam with a finer texture implies a greater reduction of gas mobility (Lake et al., 2014). In the laboratory, computed tomography (CT) has often been used to study foam flooding in core plugs (Tang et al., 2019; Gong et al., 2020). The saturation of different phases is mapped, to evaluate the performance of the foam. However, foam texture at the microscopic level is still less understood.

In this study, we present a novel technique of image analysis on foam in two 1-meter-long model fractures (analogous to microfluidic porous media). The fractures are made of glass plates (AlQuaimi and Rossen, 2018). Each model fracture has one flat wall and one rough wall. The gap between the two walls represents the aperture of the fracture. The distribution of aperture can be represented as a 2D map of pores and throats. The two fractures have different roughness distributions. One has a roughness in a regular pattern with a hydraulic aperture of 46  $\mu\text{m}$ . The other one has an irregular pattern with a hydraulic aperture of 80  $\mu\text{m}$ .

To quantify the roughness of the fractures, we profile the roughened surface (size: 2  $\times$  2 cm, resolution: 1342  $\times$  1342, pixel length: 14.9  $\mu\text{m}$ ) of the glass plate using a digital microscope. The fracture volume of the two models is also measured. The transparency of model fractures allows direct visualization of foam in the fractures, using a high-speed camera. A high-parallelism backlight is used to provide stable lumination for the camera. The whole setup is placed in a tent to avoid outside reflection and refraction.

In this study, 2D image analysis of foam is performed using ImageJ software. We characterize foam texture by quantifying bubble density, bubble size and area fraction of water and gas. We also program macros to compute the velocity of flowing bubble trains. In addition, by using profiling data, we can convert phase area fraction to 3D volume fraction. We can also estimate the capillary pressure in the model fracture. From that we can estimate the lamella surface area available for foam coarsening by gas diffusion. Based on this information we can distinguish when diffusive coarsening stops because bubble pressures are equalized or slows nearly to a stop because bubbles lose contact through lamellae.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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MS3 / 757

## A Phase-Filed-Based Formulation for Chemically-Assisted Fracture

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Predicting and controlling fractures in porous materials has posed many challenges in understanding the long-term performance of such complex systems. Geological systems such as CO<sub>2</sub> sequestration, geothermal, waste repositories, oil and gas recoveries, are examples of natural porous materials, where fracture and damage play significant roles. In many of these systems, chemical alterations lead to change in the properties of fracture as well as the mechanics of the intact porous material. This presentation focuses on fracture initiation and propagation and shows how the state-of-the-art phase-field fracture can be used to model chemically-driven fracture in porous systems. We introduce a chemical damage parameter which is coupled with mechanical damage parameter obtained from the phase-field equation. The chemical damage parameter is also coupled with the change in porosity due to dissolution occurring in the porous material. We will demonstrate how this coupled formulation enables us to gain an understanding of fracture behavior in various geological porous systems. We also discuss how chemical dissolution impacts the crack speed and directionality.

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## A Semi-Analytical Solution for Modeling of Early-Time and Late-Time Countercurrent Spontaneous Imbibition in Porous Media

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Countercurrent spontaneous imbibition (SI) is an important flow mechanism to recover oil in water- and mixed-wet porous media by means of capillary pressure. Experimental imbibition tests conducted in conventional core samples and numerical simulations show that oil recovery as a function of time occurs in a characteristic S-shaped form, which describes the infinite acting and the boundary-dominated regime. Although scaling time groups have been proposed to model SI in porous media, they fail to properly scale the results onto a single curve. Thus, the use of conventional approaches to estimate oil recovery such as an exponential model can result in wrong estimates of oil recovery.

Here, we present a new semi-analytical approach to model 1D countercurrent SI for oil-water systems through a general solution in Laplace transform of the mass-conservation equation. The infinite acting regime is modeled by a universal, early-time function that enables the accurate scaling of oil recovery onto a single curve. The early-time function considers the infinite acting behavior extends after the fluid reaches the no-flow boundary (March et al. 2016). The boundary-dominated regime is modeled by including a time-dependent diffusion coefficient into the general solution, which acts as a correction factor during the filling behavior. The Laplace transform solution is numerically inverted using the Gaver-Stehfest method. The novelty of the model is that it enables the accurate estimation of fluid imbibition under the boundary-dominated regime, a flow condition critical to evaluate the true potential of SI driven by capillarity for oil recovery in porous media. We verified the model against numerical simulations under a wide range of flow conditions relevant in water-oil systems. We show that fluid imbibition during the dominated-boundary regime is primarily driven by the diffusion coefficient and mainly affected by the viscosity ratio and the capillary pressure.

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MS3 / 266

## **A Stochastic Particle-Based Framework for Multiphase Flows in Fractured Porous Media**

**Authors:** Ranit Monga<sup>1</sup> ; Daniel W. Meyer<sup>2</sup> ; Patrick Jenny<sup>1</sup>

<sup>1</sup> *Institute of Fluid Dynamics, ETH Zürich*

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In the context of two-phase flows in porous media, Tyagi and Jenny (2008) have discussed the potential of particle-based schemes to simulate macroscale transport using the information of microscale flow dynamics. However, with the uncertainties in heterogeneity characterization and additionally, modeling challenges, obtaining a well-informed picture of microscale dynamics is not feasible. Instead, a probabilistic description can be used which focuses on the Lagrangian evolution of fluid elements and the properties associated with them, e.g., scalar concentration [Tyagi and Jenny (2011)].

In probability density function (PDF) methods, for example, computational (stochastic) particles, characterized by their position and properties, are used. Particles evolve as per stochastic processes which are defined such that the computational particles and fluid elements are statistically equivalent

[Pope (1985)]. We devise a stochastic particle framework that simulates multi-phase, multi-species transport in a fractured porous media with a permeable matrix.

We adopt an Embedded Discrete Fracture Model (EDFM) where the discretization of the matrix is independent of the fracture geometry, and the fractures are treated as lower dimensional manifolds [Hajibeygi et al. (2011), Deb et al. (2017)]. The flexibility of using a structured grid for the matrix makes EDFMs better suited for particle-based transport models. The matrix–fracture interfaces are not resolved within the grid-cells, which motivates a probabilistic description of particle transfer between the matrix and the fractures.

In Monga et al. (2020), we presented a conservative stochastic particle-tracking scheme for advective, single phase solute transport in fractured reservoirs. This scheme uses a continuous time Markov process for inter-continuum exchange, characterized by particle transfer probabilities. These probabilities depend on the particle pathline and scale with the particle's time to traverse a grid cell.

The focus of the current work is to extend the above stochastic particle scheme to model saturation evolution in a multi-phase immiscible flow. Similar to Tyagi et al. (2008), particles propagate in the physical (and property) space(s). Macroscale quantities like the saturation are defined by particle ensembles (over finite volumes). In our work, a particle has an additional attribute, i.e., its continuum state, and the transfer probabilities govern its evolution. The ensemble-derived flux is consistent with the macroscale laws for the average flux given by, e.g., Darcy's law and flux functions for fluid exchange between continua.

The hyperbolic nature of non-linear saturation transport and a finite ensemble size pose a challenge for particle methods, mainly in terms of capturing saturation discontinuities. We tackle this by adding minimal dispersion to the transport.

#### **Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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MS24 / 41

## **A Three-Scale Model for Flow in Paleo-Karst Reservoirs**

**Authors:** Marcio Murad<sup>1</sup> ; Patricia Pereira<sup>2</sup> ; Sandro Valente<sup>3</sup> ; Paola Ferraz<sup>4</sup> ; Eduardo Abreu<sup>5</sup>

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A three-scale model for flow in karst conduit networks in carbonate rocks is constructed based on a reiterated homogenization procedure. The first upscaling, performed from the high-fidelity flow model, is based on a topological model reduction considering a discrete network of conduits. The subsequent macroscopization procedure projects the reduced model into the cells of a coarse computational grid, where homogenized equivalent properties are numerically constructed. Such a two-level upscaling gives rise to a macroscopic flow model characterized by mass-transfer functions between the geological structures. A notable consequence of the approach proposed herein is the appearance of a new karst index concept, based on the generalization of the traditional Peaceman's theory of well index, along with two skin factors. The former skin is of geometrical nature, and stems from non-circular cross-section, whereas the latter captures the presence of the damage zone arising from the presence of collapsed-breccia in the vicinity of the conduit network. Computational simulations are obtained by discretizing the coupled 1D/3D flow model by a Mixed Multiscale Method in its recursive form seated on a domain decomposition approach.

#### **Time Block Preference:**

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A three-scale index for flow in karst conduits in carbonate rocks. *Advances in Water Resources* vol 141 (2020)

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MS6-B / 223

## **A Unified Gas–Alkane Binary Interfacial Tension Calculation for A Broad Range of Pressure and Temperature: A Machine Learning Approach**

**Authors:** Yingnan Wang<sup>None</sup> ; Zhehui Jin<sup>None</sup>

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Gas injection is one of the most effective enhanced oil recovery (EOR) methods, in which the gas–alkane interfacial tension (IFT) is an important parameter. Thus, to accurately estimate gas–alkane mixture IFT plays an imperative role in both chemical and petroleum engineering. Various empirical correlations by fitting the experimental results have been developed in the last several decades, which are convenient to use. However, their accuracies are inconsistent over a wide range of compositions, while some of them also need inputs from the equation of state (EOS) modeling. Statistical mechanics models and molecular simulations are other popular choices for IFT prediction, whereas they can be time-consuming. Recently, the extended Connors–Wright (ex–CW) model has been proposed to accurately predict gas–alkane IFT over a wide range of pressure, temperature, and composition. In this work, the ex–CW model is used to provide enormous IFT data to be paired with machine learning (ML) approaches to construct simple yet highly-accurate gas–alkane binary mixture IFT prediction equations (i.e. linear equations) which are functions of temperature, pressure,

and molecular weight. The linear equations for gas-alkane binary mixture IFT based on ML are calibrated by comparing with experimental data, the ex-CW model, and the Parachor model. We find that the linear equations from ML approach largely outperforms the Parachor model, while they have a comparable performance with the ex-CW model. In addition, while both the Parachor model and the ex-CW model need the inputs from the EOS modeling, the linear equations from ML approach only use temperature, pressure and molecular weight. The proposed idea shows a great potential in terms of highly-efficient and highly-effective gas-alkane binary mixture IFT predictions which can be further extended to more-complicated multi-component gas-oil IFT predictions for gas injection EOR processes.

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MS13 / 189

## A Unified Plot for Fluid Phase Transitions

**Authors:** Henry Enninful<sup>1</sup> ; Dirk Enke<sup>2</sup> ; Rustem Valiullin<sup>3</sup>

<sup>1</sup> *Universität Leipzig*

<sup>2</sup> *Leipzig University*

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While many mesoporous materials are found naturally (clays, coal, and shale), many others are synthesized for industrial applications like sensing, fluid separations, and energy storage. For the optimization of these materials for various applications, an accurate determination and understanding of the pore size distribution and morphology is vital.

Fluid phase transitions employ the alteration of physical properties of confined fluids as markers for pore space characterization. This is expressly revealed by the Kelvin equation for gas-liquid transitions and the Gibbs-Thomson equation for solid-liquid transitions. As may be thought, for one and the same material, both methods are expected to yield the same pore size distribution with little or no deviations. However, it has been shown that, both approaches may yield slightly different results.

Herein, we introduce a unified plot for both gas-liquid and solid-liquid transitions based on the Kelvin and Gibbs-Thomson equations. We analyze three mesoporous silica solids; SBA-15, Vycor and MCM-41, in order of decreasing pore size. Remarkable similarity is observed in the fluid phase transitions in the SBA-15 material of pore size approximately 9nm. With decreasing pore size, a divergence between both transitions is observed. We postulate that, this may primarily be due to the increasing influence of thermodynamic fluctuations with decreasing pore size.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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MS3 / 515

## A Virtual Element Discretization of a 3D Elastoplastic Problem

**Author:** Francesca Marcon<sup>1</sup>

**Co-authors:** Andrea Borio<sup>1</sup> ; Stefano Berrone<sup>2</sup>

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In order to model mechanics of porous media, the elastoplastic behaviour of materials, such as rocks and soils, plays an important role. In this work, we study Virtual Element Methods for 3D elastoplastic simulations. We focus on the equations that characterize the elastoplastic 3D model in the framework of small deformations theory. We especially deal with the Mohr-Coulomb plasticity model, which is suited to describe the plasticity behaviour of materials in which we are interested. We apply its yield function and flow potential to define associative and non associative plasticity. Due to numerical problems of the model, we study and implement a 'smooth' version of the Mohr-Coulomb model, proposed by Abbo and Sloan (2011). This aspect requires the study of a suitable generalized Return Mapping Algorithm. Moreover, we have to tackle with a strong non-linearity involved in the model. This issue requires the study and the application of a proper globalization strategy for Newton method, for instance line search methods. Furthermore, as regards the variational discretization framework, we focus on the VEM formulation of the 3D primal elastoplastic equation, combined with the stress estimation through the Return Mapping Algorithm. We study a suitable stabilization for the problem with respect to the one introduced by Beirão da Veiga et al (2015). Finally, we present a 3D numerical experiment of limit analysis on slope stability, which is a classical benchmark problem for Mohr-Coulomb plasticity model, and other results in order to discuss numerical problems of the model and the strategies to deal with them.

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Time Block A (09:00-12:00 CET) **References:**

Abbo, A.J. and Lyamin, A.V. and Sloan, S.W. and Hambleton, J.P. 2011 A C2 continuous approximation to the Mohr-Coulomb yield surface. *International Journal of Solids and Structures* 48, 3001-3010

Beirão da Veiga, L. and Lovadina, C. and Mora, D. 2015 A Virtual Element Method for elastic and inelastic problems on polythope meshes. *Comput. Methods Appl. Mech. Engrg.* 295, 327-346 **Acceptance of Terms and Conditions:**

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## A chronopotentiometric study of polymeric ion-exchange membranes in alcohol-water media

**Authors:** David García-Nieto<sup>None</sup>; Juan Carlos Maroto<sup>1</sup>; Sagrario Muñoz<sup>2</sup>; V. María Barragán<sup>3</sup>

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Chronopotentiometry is a powerful technique to investigate transport phenomena in charged porous medium-electrolyte interfaces, especially those associated with ion transport in the overlimiting regime. It allows to determine the transition time, which is an important characteristic of transient ion transport. Under certain conditions, the Sand equation can be applied to analyse fouling effects, the inhomogeneity of the surface or to determine ion transport numbers in polymeric ion-exchange membranes. Even ion-exchange membranes based on chemically homogeneous polymers can exhibit microheterogeneities disturbing the ion transfer. The surface heterogeneity of the membranes used in many electrochemical systems is an important issue and it has been actively studied, but usually aqueous electrolyte systems have been studied.

In this work we apply chronopotentiometry for studying polymeric ion-exchange membranes in alcohol-water media. A non-reinforced homogenous membrane, Nafion 117, and two reinforced homogeneous membranes, Neosepta CMX and AMX, have been investigated in LiCl 0.005 M electrolyte solutions with 2M alcohol-water solution as solvent. Methanol and ethanol were used as alcohols. Limiting current values were determined from voltage-current curves. The transition times were obtained as a function of the density current and the agreement with the Sand theory has been analysed.

Financial support from Banco de Santander and Universidad Complutense de Madrid is gratefully acknowledged.

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MS8 / 530

## A detailed pore scale modelling of colloid transport in porous media using lattice Boltzmann method

**Authors:** Mandana Samari Kermani<sup>1</sup>; Saeed Jafari<sup>2</sup>; Mohammad Rahnama<sup>2</sup>; Amir Raoof<sup>3</sup>

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### Abstract

A fully coupled pore scale model was developed with the aim of exploring the effects of hydrodynamic forces, ionic strength, and zeta potential on colloids transport under both favourable and unfavourable conditions. The Lattice Boltzmann-Smoothed Profile method was used to simulate

particle-particle and particle-fluid interactions without a need for assumptions of dilute suspension and clean bed filtration. Simulation using a wide range of parameters have shown creation, and breakup of agglomerates. Results are used to obtain time-averaged behaviour of transport properties, such as pore void fraction, conductivity, and surface coverage. We have found that in comparison with zeta potential, increasing ionic strength had a greater impact on particles behaviour. A raise in ionic strength, and a decrease in flow velocity caused a decrease in pore void fraction and its conductivity and an increase in aggregates connectivity.

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## **A digital workflow for analysis of flow in porous media: Multi-phase transport phenomena from pore to field scale in subsurface flow**

**Author:** Thomas Ramstad<sup>1</sup><sup>1</sup> *Equinor***Corresponding Author:** trams@equinor.com

Multiphase flow in porous media is strongly influenced by the pore-scale mechanisms and in-situ arrangement of fluids. How fluids are distributed and transported are dependent on the pore structures in addition to wettability, fluid-fluid interactions and external boundaries. It is essential to understand these pore scale effects to obtain good constitutive relations for characterization of subsurface flow on multiple length scales.

To better predict fluid transport in subsurface reservoirs, the subsurface industry relies heavily on analysis of reservoir rock core materials and fluids. By leveraging advances in pore scale imaging technology, we now frequently use high resolution X-ray computed tomography (CT) and micro-CT to get insight in fluid distribution and transport directly inside the pore space. Combined with core flooding experiments, such imaging capabilities may greatly enhance the value of experimental analysis and pore scale modelling.

I will in this talk present development of a workflow that combines core flooding experiments with CT imaging and pore scale modelling. Small samples of rock material are scanned with in-house micro-CT / CT equipment to generate 3D images of pore space and fluid distribution with resolutions down to a few micrometers. Sophisticated image analysis tools are used to acquire and register multiple scans of a sample, so that we can directly compare changes to fluid arrangements. Ultimately, digital pore scale models are generated for simulations of two-phase flow.

By collecting results from the different steps in such a digital workflow, we have gained new knowledge about pore scale transport mechanisms. That is again used to supplement results from traditional special core analysis (SCAL) such as capillary pressure, relative permeability curves and end-point saturations. Such parameters are essential input to large scale reservoir models used to improve drainage strategy, geologic carbon storage and enhance petroleum recovery.

Advances in knowledge of flow in porous media rely on a close collaboration between industry, vendors and academia. We continuously strive to improve and develop our analysis and software toolbox. The rapid evolution of open source development has created additional platforms for direct research collaboration between academia and industry, and faster deployment of novel research results.

One such platform that we are involved in, is the Open Porous Media (OPM) project, which contains several open source tools for modelling and upscaling flow in porous media. I will present some of them, and how these are used actively in our research.

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## A discrete element model (DEM) for swelling behavior of clay

**Authors:** Srutarshi Pradhan<sup>1</sup> ; Martin Alexander Toresen<sup>2</sup>

<sup>1</sup> *Researcher, PoreLab, NTNU*

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Swelling of Shale-rocks create several problems [1] during underground drilling operations, such as stuck-pipe/drill-bit. However, swelling of shale-rocks can close the gaps between rock (wellbore) and casing –therefore no cementing is needed – which can save a lot of time and money and such a “natural” closing ensures “no-leakage” during further drilling and production phases. The field experience reveals that some shale-rocks are good candidate for swelling and some are not. It is believed that, amount of clay is the most important factor for shale-swelling. There are several other parameters that can influence the swelling behavior, such as- porosity, quartz contents, clay-cluster distribution, stress difference between field and drilling zone etc. Therefore, to plan a safe and efficient drilling through shale-rocks, we should understand the swelling mechanism of clay.

To investigate swelling of clay, we have introduced a discrete element model (DEM), based on Monte-Carlo technique. We define a probability of swelling for all the clay grains in the shale-rock sample that includes the effect of stress-difference, porosity, temperature etc. The time evolution of grain swelling results in bulk swelling behavior of the sample and the simulation result qualitatively matches [2] with the observations of shale/clay swelling experiments [3,4]. The Monte-Carlo based DEM code has been studied [5] for the entire parameter space by varying several important inputs like porosity, clay-quartz contents, stress difference, temperature etc. In addition, the mass-transport phenomenon has been implemented by considering clay grain movement through fractures (flow channels).

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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5. M. A. Toresen, Master thesis on “Computational Modelling of Clay Swelling” 2020-2021, Physics Department, NTNU, Trondheim. **Acceptance of Terms and Conditions:**

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Poster + / 303

## A dynamic pore network model for imbibition simulation considering corner flow

**Authors:** Jianlin Zhao<sup>1</sup> ; Feifei Qin<sup>2</sup> ; Qinjun Kang<sup>3</sup> ; Dominique Derome<sup>4</sup> ; Jan Carmeliet<sup>5</sup>

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Wetting films can develop in the corners of pores in porous media under strong wetting conditions where the contact angle allows the wetting phase to invade the corner. Such corner flow has a significant influence on the two-phase flow dynamics. Compared with the main meniscus rising within a pore, the wetting corner film is much thinner and can lie significantly ahead. Modeling the dynamics of corner film remains elusive using direct numerical simulation method because of the significant scale difference between main meniscus flow and corner film flow. In this presentation, we propose a dynamic pore network model for imbibition simulation which can accurately account for corner flow. First, a modified interacting capillary bundle model is presented to describe the liquid imbibition dynamics in a single angular tube with corner films. In this model, a square tube is decomposed into several interacting sub-capillaries with the first sub-capillary representing the main meniscus and the other ones representing the corner films. The conductance of each sub-capillary is calculated based on single-phase lattice Boltzmann simulation. The modified interacting capillary bundle model is validated by comparing its results with the two-phase lattice Boltzmann simulation results for the same geometry. Then this modified interacting capillary bundle model is incorporated into a dynamic pore network model with single-pressure algorithm. Thus the pore network is decomposed into several layers of interacting sub-pore-networks where the first layer of sub-pore-network simulates the main meniscus flow in the porous media while the other sub layers simulate the corner film flow. The snap off mechanism is also introduced into the model, which plays an important role under low flow rate condition. Finally, both the proposed dynamic pore network model and a two-phase lattice Boltzmann model are used to simulate wetting fluid redistribution in a porous medium induced by capillary force and corner film flow. The good agreement between the simulation results of both methods demonstrates the accuracy of the proposed dynamic pore network model in considering corner flow.

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## A framework to map pore volume change and mineral dissolution/precipitation of wellbore cement exposed to high concentration CO<sub>2</sub> using micro-CT images

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In this study, an image processing framework was proposed for mapping Ca(OH)<sub>2</sub> dissolution, CaCO<sub>3</sub> precipitation, and pore volume change of wellbore cement samples exposed to high concentration CO<sub>2</sub> under laboratory-simulated geologic CO<sub>2</sub> storage conditions. The main workflow covered in this framework is to, 1) remove noises, artifacts, beam hardening effects, etc. from micro-CT images of cement samples before and after reaction with CO<sub>2</sub>; 2) register cement CT images before and after reaction; 3) generate grayscale intensity difference images showing CO<sub>2</sub>-induced cement alteration, and convert grayscale intensity difference into X-ray attenuation coefficient change; 4) calculate pore volume change and local content changes of Ca(OH)<sub>2</sub> and CaCO<sub>3</sub> at each voxel, given X-ray attenuation coefficient change; 5) generate pore volume change and Ca(OH)<sub>2</sub>/CaCO<sub>3</sub> content changes in 3D view. The effectiveness of the framework was validated through a step-by-step demonstration of results when deploying the framework to process the micro-CT images of six cement samples acquired before and after reaction with CO<sub>2</sub>. The 3D CaCO<sub>3</sub> precipitation and Ca(OH)<sub>2</sub> dissolution map was obtained, and the internal and external CaCO<sub>3</sub> shells were visualized. Overall, the 3D precipitation and dissolution map gives more intuitive and interpretable results of CO<sub>2</sub>-induced alteration of cement than the direct visual comparison from original CT images.

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MS9 / 166

## A fully parallel Pore Network Simulator for plug size pore scale simulations

**Authors:** Mohamed Regaieg<sup>1</sup> ; Clément Varloteaux<sup>2</sup> ; Arthur Moncorgé<sup>1</sup> ; Titly Farhana Faisal<sup>3</sup> ; Igor Bondino<sup>1</sup>

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Pore scale simulation is increasingly used to study various phenomena that cannot be reproduced by conventional Darcy-based simulators. Direct Numerical Simulation (DNS) on systems larger than few millimeters is too computationally demanding. Pore Network Modeling (PNM) is a practical way to study the flow at pore scale on larger volumes while keeping reasonable running times.

Recent advances have improved the speed of Pore Network Models (Regaieg et al, 2017, Petrovsky et al, 2020), while interesting speed-ups have been achieved, they are still not enough for tens of million pores simulations and memory starts to become the limiting factor. In order to accelerate our pore network simulations and to overcome memory limitations, we propose TOTAL's fully parallel pore network simulator DynaPNM used in quasi-static mode.

In this talk, we first describe the parallel pore network simulator. Then, we present several test cases where we show that this parallelization improves the computational performance without losing the accuracy of the solution. All the simulations were run on TOTAL's supercomputer PANGAEA on networks of real rocks. Each network represents an upscaled version of the 3D segmented image of the rock in the form of a network of pore elements where the single-phase flow conductances in each pore are derived by solving the Stokes equation in the original geometry (Raeni et al, 2017). The extraction of large volumes became possible using a newly developed stitching algorithm (Varloteaux et al, 2021).

We then describe how simulation runs in parallel mode allow to perform large uncertainty studies (thousands simulations / day) on networks extracted from images that represent a size as large as (10000x8000x8000) voxels representing a rock volume of 46 cm<sup>3</sup> which is a typical size of a plug used in capillary pressure measurements. We document the very large statistical dispersion in relative permeability results (due to the microscopic arrangement of oil-water contact angles) that is normally achieved when images as small as 1000x1000x1000 are used in simulation. We show how this finite size effect can be drastically reduced by simulating much larger and representative images, greatly improving the precision of the numerical result.

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## A homogenised model for flow, transport and sorption in a heterogeneous porous medium

**Authors:** Lucy Auton<sup>1</sup> ; Satyajit Pramanik<sup>1</sup>

**Co-authors:** Chris MacMinn<sup>1</sup> ; Mohit Dalwadi<sup>1</sup> ; Ian Griffiths<sup>1</sup>

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A major challenge in flow through porous media is to better understand the link between pore-scale microstructure and macroscale flow and transport. For idealised microstructures, the mathematical framework of homogenisation theory can be used for this purpose. Here, we consider a two-dimensional microstructure comprising an array of circular obstacles, the size and spacing of which can vary along the length of the porous medium. We use homogenisation via the method of multiple scale to systematically upscale a novel problem that involves cells of varying area to obtain effective continuum equations for macroscale flow and transport. The equations are characterized by the local porosity, an effective local anisotropic flow permeability, and an effective local anisotropic solute diffusivity. These macroscale properties depend non-trivially on both degrees of microstructural geometric freedom (obstacle size and spacing). We take advantage of this dependence to compare scenarios where the same porosity field is constructed with different combinations of obstacle size and spacing. For example, we consider scenarios where the porosity is spatially uniform but the permeability and diffusivity are not. Our results may be useful in the design of filters, or for studying the impact of deformation on transport in soft porous media.

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## A hybrid-dimensional compositional two-phase flow model in fractured porous media with phase transitions and Fickian diffusion

**Authors:** Joubine Aghili<sup>1</sup> ; Jean-Raynald de Dreuzy<sup>2</sup> ; Roland Masson<sup>3</sup> ; Laurent Trenty<sup>4</sup>

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We consider an extension of Discrete Fracture Matrix (DFM) models to compositional two-phase Darcy flows in fractured porous media.

The model is hybrid-dimensional, i.e. fractures are treated as surfaces of co-dimension one, and accounts for phase transitions and Fickian diffusion. It is based on physically consistent transmission conditions across matrix fractures (m-f) interfaces resulting from flux continuity equations at interfaces and Two-Point Flux Approximations in the fracture width. They allow to capture saturation jumps for general capillary pressure laws as well as the Fickian diffusion in the fracture width and the thermodynamical equilibrium based on complementary constraints. DFM models introduced previously consider simplified transmission conditions at m-f interfaces classically obtained by jumping over the m-f interfaces in order to reduce the computational cost. However, we show that they are less accurate than our reduced model and leads, in some cases, to physically inconsistent solutions. Validation is made with a reference equi-dimensional model.

We will also show that the Fickian diffusion plays a crucial role on the gas transfer at the m-f interfaces. This point will be discussed and illustrated with two types of test cases both using a fluid system with liquid and gas phases defined as mixtures of air and water components. Finally, we investigate the desaturation by suction with a data set based on Andra nuclear waste storage prototype facility.

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MS9 / 66

## A level set approach to Ostwald ripening of real gases in porous media

**Authors:** Deepak Singh<sup>1</sup> ; Helmer André Friis<sup>2</sup> ; Espen Jettestuen<sup>2</sup> ; Johan Olav Helland<sup>3</sup>

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Ostwald ripening phenomenon is particularly important for foam EOR and geological CO<sub>2</sub> storage projects where coarsening can lead to increased mobility of isolated gas bubbles. It is a thermodynamic process by which bubbles in bulk foam coarsen with bigger bubbles growing at the expense of smaller bubbles. Previous studies in literature have shown that in porous media this gas phase interaction is more complicated and bubble growth depends on the bubble interfacial radius (or pressure) rather than size. However, research on Ostwald ripening in porous media is generally carried

out with a notable assumption that the pressure of fluid in contact with gas phase is constant. In porous media, fluid phase pressure varies during flow through pores and pore throats which in turn should affect the pressure and interfacial radius of gas bubbles. This makes it imperative to study the phenomena considering isolated fluid ganglia in contact with gas bubbles.

In this work, we have used a multiphase local volume conserved level-set method based on SAMRAI framework (Jettestuen et al., 2021) to model Ostwald ripening process in porous media. The approach is based on the ghost bubble method proposed by Lemlich(1978) to characterize fluid phase interactions in wet foam. We suggest chemical potential difference instead of pressure difference as the driving force behind mass transfer. This approach directly links the mass transfer to Gibbs energy potential of the bubbles. The method is validated for two-phase systems interacting within pore space with results from deChalendar et al. (2018). Our pore scale model is compatible with parallel programming and can be used to carry out studies on large computational grids. The model can also incorporate different wettability states of the porous media using different phase contact angles.

Comparative study was carried out between Soave-Redlich-Kwong (SRK), Van der Waals' (VdW) and Ideal gas equation of state to study the effect of using ideal gas assumption. The equations of state were used to calculate fugacity of gas in isolated bubbles at different pressures and reservoir temperature. The gas bubble fugacity was used to determine their chemical potential. The model was also used to study mobilization of an isolated bubble in a microchannel due to Ostwald ripening from smaller bubbles in adjoining pore space. We have also studied the effect of local capillary pressure on gas bubble stability. Finally, we show how Ostwald ripening impacts residual two-phase fluid configurations in a 3D sandstone pore geometry after waterflooding. We quantified the evolution of pressure, volume and area relationship, for residual bubbles.

One significant result of our work is that presence of an isolated fluid phase between two gas bubbles can limit coarsening and stabilize small gas bubbles in porous media. Another important result is that it shows that use of ideal gas equation underpredicts the rate of coarsening.

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Time Block B (14:00-17:00 CET) **References:**

de Chalendar, J.A., Garing, C., & Benson, S.M. (2018). Pore-scale modelling of Ostwald ripening. *J. Fluid Mech.*, 835, 363-392. DOI: <https://doi.org/10.1017/jfm.2017.720>

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## A macroscopic two-length-scale model for natural convection in porous media driven by a species-concentration gradient

**Author:** Stefan Gasow<sup>1</sup>

**Co-authors:** Yan Jin<sup>1</sup> ; Marc Avila<sup>1</sup> ; Andrey V. Kuznetsov<sup>2</sup>

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Turbulent natural convection in porous media has received increasing attention in recent years, especially due to its significance in emerging engineering applications, such as the long-term storage of

CO<sub>2</sub> in deep saline aquifers or thermal-energy storage systems. Macroscopic equations are usually solved to calculate natural convection in porous media. The numerical solution of volume-averaged Darcy-Oberbeck-Boussinesq (DOB) equations is the most common macroscopic approach, but the DOB equations only account for the microscopic properties of the porous medium via the permeability and effective diffusivity. This simplification may be the reason for the discrepancies between the Sherwood/Nusselt number scaling from DOB simulations and laboratory experiments.

We performed pore-scale-resolving direct numerical simulations (DNS) of turbulent natural convection in a porous medium (Gasow *et al.* 2020). Our DNS results lead to the conclusion that two length scales (the pore scale and the characteristic macroscopic length scale) and the viscous diffusion term, should be explicitly accounted for in the macroscopic equations. Because the DNS results showed that the viscous diffusion term is of the same order of the Darcy number ( $Da$ ) as well like the buoyancy force term and the Darcy term.

Based on our analysis, we proposed a new macroscopic model the two-length-scale diffusion (TLSD) model, where we assume that pore scale structures affect the momentum transport through macroscopic diffusion. Whereby the macroscopic diffusion is determined by the two length scales, the pore size characterized by the square root of the permeability and the characteristic macroscopic length scale, which is the distance between the lower and upper boundaries.

The results of this model were validated with our DNS results, which were volume-averaged over each representative elementary volume (REV) of the porous medium to obtain the respective macroscopic fields. The comparison shows that our proposed macroscopic model is more accurate than the traditional DOB model and performs well as long as  $Da > 2 \times 10^{-6}$ . In particular the new model can predict well the phenomenon revealed by our DNS results that the Sherwood ~ Rayleigh number scaling changes from a linear scaling to a non-linear scaling as the porosity increases. The new macroscopic model also predicts well that if the Rayleigh number is fixed, the Sherwood number increases with the increase of the Schmidt number and the decrease of the porosity. These trends agree with the DNS results, whereas they cannot be captured by the DOB simulations.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

Gasow, S., Lin, Z., Zhang, H. C., Kuznetsov, A. V., Avila, M. & Jin, Y. 2020 Effects of pore scale on the macroscopic properties of natural convection in porous media. *J. Fluid Mech.* 891, A25 **Acceptance of Terms and Conditions:**

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## A midsurface extraction framework applied to core sample images for dimension reduction of fracture objects

**Author:** Carlos Augusto Soares Ferreira<sup>1</sup>

**Co-author:** Hamid M. Nick<sup>2</sup>

<sup>1</sup> Danish Hydrocarbon Research and Technology Centre

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The modelling of multiphase flow and mechanical response in fractured chalk formations due to oil and gas exploitation is of major importance in the understanding of the subsurface processes and the environmental impact associated with such activities. In addition, this knowledge is highly essential to predict unwanted effects from future carbon capture and storage (CCS) practices [1-3] and geothermal applications [4-6]. On the modelling of the fractures in porous media there are basically two classes of methods: (a) continuum methods [7-9] (or implicit methods), in which fractures and

porous matrix are represented by two overlapping continua and a transfer function is used to model the interaction between these two, and (b) discrete methods [10–13] (or explicit methods), in which two different grids are used for fractures and porous matrix and the interplay between these two is represented explicitly. Employing a discrete method allows a more accurate representation of the fractures and subsequently the interplay between these and the porous matrix, but at the expense of a larger computational cost. The continuum approach presents a much lower computational cost. However, the existence of a representative elementary volume (REV) and accurate homogeneous parameters cannot be guaranteed [14]. Furthermore, previous works have shown that averaging the heterogeneous aperture to scale up permeability results in an underestimated fluid flow pattern [15], indicating the necessity of incorporating full aperture distributions rather than simplified aperture representations in reservoir-scale flow models [16–18]. Given the importance of the fractures modelling for accurate predictions of the fluid flow patterns and the extra cost involved in employing a discrete method, mixed-dimensional models [10,12,19], in which porous matrix is modelled as a  $d$ -dimensional entity, whereas fractures are modelled as  $(d - 1)$ -dimensional entities, were developed aiming a cheaper but accurate framework. This work explores the reduction of two-dimensional fracture objects obtained from images to one-dimensional objects, such that a mixed-dimensional model might be employed. A skeletonization technique [20] along with a skeleton network generation [21] are employed for extraction of the one-dimensional fracture object, while medial axis [22] is used for aperture distribution calculation. The mesh generated through this framework is used in numerical simulations carried with the mixed-dimensional model for fluid flow in fractured porous media.

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## A mixed-dimensional model for thermo-chemical-flows in fractured porous media

**Authors:** Anna Scotti<sup>1</sup> ; Alessio Fumagalli<sup>1</sup>

<sup>1</sup> *Politecnico di Milano*

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In this presentation we introduce an innovative mathematical model that is able to describe chemical processes that may occur in fractured porous media. A solute is carried by a fluid in the porous medium, that reacting precipitates forming a salt that might alter the physical properties of the system, creating zone of low flow. Conversely, if the salt dissolves it might open up new pathways especially through previously clogged fractures. These chemical reactions depends also on the temperature, which controls their speed. We consider thus a fully-coupled and non-linear system of mixed-dimensional equations that is able to describe such phenomena. Numerical examples show the applicability of the proposed model.

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## A modified pulse-decay approach to simultaneously measure permeability and porosity of tight rocks

**Author:** Yue Wang<sup>1</sup>

**Co-authors:** Bernhard KROOSS<sup>2</sup> ; Moran Wang<sup>1</sup> ; Steffen Nolte<sup>2</sup>

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Permeability and porosity are two most important parameters of rocks for evaluation and exploitation of oil/gas reservoirs. In this study, a modified pulse-decay method has been developed to measure both permeability and porosity simultaneously. In the proposed method, the gas pressure in one chamber is changed (increased or decreased) instantaneously and then maintains constant, while the pressure response changing with time in the other one is monitored. A mathematical model of this procedure has been formulated, and a general analytical solution has been obtained. The late-time solution is presented for post processing of experimental data, which leads to measurements of permeability and porosity values of tight rocks simultaneously. Our measurements agree well with those from the classical pulse decay and gas expansion methods. The proposed method can reduce the total test time and ensure the permeability and porosity are measured under the same effective stress condition.

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## A multiscale approach for the characterization of bio-chemo-mechanical processes in contaminated marine sediments

**Authors:** Claudia Vitone<sup>1</sup> ; Francesca Sollecito<sup>2</sup> ; Federica Cotecchia<sup>1</sup> ; Alexander Puzrin<sup>3</sup> ; Michael Plötze<sup>3</sup> ; Rossella Petti<sup>1</sup>

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The research has been stimulated by the emblematic case of the Mar Piccolo, in the city of Taranto (South of Italy). It is a heavily polluted marine basin but, at the same time, it hosts unique natural ecosystem and several protected species. The need of tuning customized and efficient remediation strategies stirred a cutting-edge multidisciplinary investigation campaign and an advanced integration of data among geologists, geophysicists, biologists, chemists, hydrogeologists, geochemists, mineralogists, geotechnical engineers and environmental technologists. They jointly designed sampling procedures, devices, sediment handling procedures, in order to ensure their compliance with the relevant standards for the different scientific fields. Thereafter, the whole team ended up with the definition of an advanced conceptual site model that included such holistic site characterisation to originally support decision makers in the risk management of the site.

The multidisciplinary investigation has produced a huge database, allowing for a new insight into the processes occurring in natural marine sediments including anthropic and natural contaminants (Cotecchia et al., 2020). In particular, the geotechnical characterisation of the clayey sediments has shown that their physical and mechanical properties do not appear to vary solely with the mineralogical composition of the soil skeleton and the depositional loading history (Sollecito et al., 2019; Vitone et al., 2020). This finding has inspired a multiscale testing on sediments, which entails understanding the extent to which either anthropogenic or natural factors trigger bio-chemo-mechanical processes that affect the geotechnical properties of marine sediments and may make the design of remedial measures particularly challenging.

Indeed, according to the Gouy-Chapman diffusive double layer model (Gouy, 1910; Chapman, 1913), the thickness of the diffusive double layer (DDL) in clay microstructure decreases when either the electrolyte concentration or the cation valence increases and the dielectric constant decreases, as

in the case of pore water including high concentrations of salts, metal ions and organic pollutants. These conditions favour flocculation and prompt significant variations in soil properties (index properties and mechanical parameter values) with respect to those exhibited by the clay including pure water. However, differently from the literature contributions dealing with spiking tests on monomineralic fine soils artificially contaminated in laboratory until fully saturated, contaminated marine sediments in natural deposits are usually formed by a pool of minerals (e.g. illite, smectite, kaolinite) and contain anthropogenic compounds (heavy metals ions and organic pollutants) that, although exceeding the environmental law thresholds, are often in diluted concentrations. Furthermore, they include several sources of natural contaminants (salinity, organic matter, diatoms, fossils) which may activate bio-geo-chemical processes.

In the case of this site, while the prime suspect for unconventional behaviour was the chemo-mechanical coupling between soil skeleton and contaminants, the innovative interpretation of thermogravimetry tests on samples of marine sediments, associated to other micro-scale tests (scanning electric microscopy and mercury intrusion porosimetry) and chemical tests, provided evidences that the biogeochemical degradation of organic matter and the presence of microfossils and diatoms is likely to affect significantly the micro to macro behaviour of contaminated marine sediments.

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## A multiscale mixed finite element method applied to the simulation of two-phase flows

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The multiscale hybrid mixed finite element method (MHM-H(div)), previously developed for Darcy's problems, is extended for coupled flow/pressure and transport system of two-phase flow equations on heterogeneous media under the effect of gravitational segregation. It is combined with an implicit transport solver in a sequential fully implicit (SFI) manner. The MHM-H(div) method is designed to cope with the complex geometry and inherent multiscale nature of the phenomena. The discretizations are based on a general domain partition formed by polyhedral subregions, where a hierarchy of meshes and approximation spaces are considered. The multiscale approach is applied to the flux/pressure kernel making use of coarse scale normal fluxes between subregions (trace variable). The fine-scale features inside each subregion are determined by resolving completely independent local Neumann problems, the boundary conditions being set by the trace variable, by the mixed finite element method using fine flux and pressure representations. These properties imply that the

MHM-H(div) can be interpreted as a classical mixed formulation of the model problem in the whole domain, based on a H(div)-conforming space with normal components over the macro-partition interfaces constrained by the trace space, and showing divergence compatibility with the pressure space [1]. Consequently, local mass conservation is observed at the micro-scale elements inside the subregions, an essential property for flows in heterogeneous media, and divergence-free constraint strongly enforced for incompressible flows. The efficient use of static condensation leads to a global system to be solved only in terms of primary degrees of freedom associated with the trace variable and of a piecewise constant pressure for each subregion. An iterative coupling technique is adopted to solve the two-phase flow equations. The numerical examples show that the proposed scheme is able to solve coupled flow and transport problems.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

[1] O. Duran, P. R. B. Devloo, S. M. Gomes, F. Valentin, A multiscale hybrid method for Darcy's problems using mixed finite element local solvers, *Computer Methods in Applied Mechanics and Engineering* 354 (2019) 213–244.

URL <https://doi.org/10.1016/j.cma.2019.05.013> **Acceptance of Terms and Conditions:**

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## A new discrete fracture model for fluid flow based on phase field method

**Author:** Qingdong Zeng<sup>1</sup>

<sup>1</sup> *Shandong University of Science and Technology*

**Corresponding Author:** [upc.zengqd@163.com](mailto:upc.zengqd@163.com)

Fluid flow in fractured porous media is a common phenomenon in many engineering applications, and many numerical methods have been proposed to capture these processes. Here, a new discrete fracture model based on phase field method is presented. The common discrete fracture models represent fractures by sharp topology in an explicit way, regardless of using conforming or non-conforming mesh. Inspired by the definition of crack phase field, the sharp fracture topology is treated as a diffusive one in the solution of fluid flow problems, and the integration of fluid flow equation over fractures can be transformed to the one over the matrix. The algorithm to determine the fracture phase field and finite element discretization are described in detail. The performance of the proposed method is validated against the classic discrete fracture model on several numerical cases in both two and three dimensions. The convergency behavior of the proposed method is furtherly investigated through sensitivity analysis to mesh resolution and fracture parameters. Numerical results demonstrate that the proposed method is accurate, convergent and quite promising for simulating fluid flow in fractured porous media.

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## A new pore-merging method for simulating mineral dissolution in porous media using pore-network models

**Authors:** Barbara Esteves<sup>1</sup> ; Paulo Laranjeira da Cunha Lage<sup>2</sup> ; Paulo Couto<sup>3</sup> ; Anthony Kovscek<sup>4</sup>

<sup>1</sup> *Stanford University / Universidade Federal do Rio de Janeiro*

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This study proposes and demonstrates a new pore-network modeling approach to simulate single-phase reactive transport and mineral dissolution in porous media. A new algorithm for the merging of pores and throats resulting from solid dissolution is introduced to guarantee the conservation of the main variables of interest during the merging process. Pore surface areas and throat conductances are modeled accurately using a novel application of correction factors and effective properties. Hence, the main objective of this presentation is to discuss this novel merging methodology and some applications in regular and random pore-network models. Our approach solves a coupled transport and reaction pore-network model that implements a kinetic model with a single heterogeneous chemical reaction describing the dissolution of calcite by acidic solutions. The reactive transport problem is described by the acid advection-diffusion transient equation in control volumes represented by pores and throats. The network geometry is updated based on the dissolution process happening at the mineral surface. Pores and throats are enlarged due to mineral consumption. The merging method is performed when two connected pores reach each other. Pore spaces are relocated in the network and correction factors are updated to conserve the effective surface areas and effective conductance of throats. The fluid flow field is also updated due to these new larger sizes of pores and throats. A wide range of pore-network models are used to study the reactive transport problem. The main results include the exploration of different dissolution regimes through porosity-permeability evolution curves, acid concentration profiles, and the use of statistical criteria to differentiate regimes. Importantly, this methodology has the ability to simulate permeability increases larger than 100-fold during the formation of preferential pathways through the network. The innovative approaches presented may be used to improve the representation of many subsurface applications where reactive transport and mineral dissolution are the fundamental phenomena at the pore-scale, including performance of acidizing for stimulation, geological storage of carbon dioxide ( $CO_2$ ), and enhanced oil recovery.

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MS9 / 236

## A new probabilistic nucleation model to predict crystal growth in porous medium

**Authors:** Mohammad Masoudi<sup>1</sup> ; Mohammad Nooraiepour<sup>2</sup> ; Andreas Berntsen<sup>3</sup> ; Helge Hellevang<sup>4</sup>

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Nucleation is the first step of any mineral precipitation and crystal growth process. It is often overlooked in studying the reactive transport phenomena. Nucleation controls the location and timing of crystal formation in a porous structure. The spatial distribution of stable secondary nuclei is crucial to predict hydrodynamics of the porous medium after mineral precipitation precisely. To better understand the nucleation process, we developed a new probabilistic nucleation approach in which the induction time is considered a random variable. The random induction time statistically spreads around the measured or reported induction time, either obtained from experiments or approximated by the exponential nucleation rate equation suggested by the classical nucleation theory. In this work, we utilized inputs from the classical nucleation theory. In our model, both location and time of nucleation are probabilistic, affecting transport properties in different time- and length-scales. We developed a pore-scale Lattice Boltzmann reactive transport model and implemented the new probabilistic nucleation model to investigate the effect of nucleation rate and reaction rate on the extent, distribution, and precipitation pattern of the solid phases. The simulation domain is a 2D substrate with an infinite source of the supersaturated solution. We use Shannon entropy to measure the disorder of the spatial mineral distributions. The results of the simulations show that all the reactions follow similar random behavior with different Gauss-Laplace distributions. The simulation scenarios start from a fully ordered system with no solid precipitation on the substrate (entropy of 0). Entropy starts to increase as the secondary phase precipitates and grows on the surface until it reaches its maximum value (entropy of 1). Afterward, the overall disorder declines as more surface areas are getting covered, and eventually, entropy approaches a constant value. The research results indicate that the slower reactions have longer windows of the probabilistic regime before entering the deterministic regime. The outcomes provide the basis for implementing mineral nucleation and growth for reactive transport modeling across time-scales and length-scales.

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## A numerical study on the role of the slight compressibility on viscous fingering

**Authors:** Fatemeh Bararpour<sup>None</sup> ; Mozhdeh Sajjadi<sup>1</sup>

<sup>1</sup> Assistant Professor

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Analyzing interfacial phenomena like Viscous Fingering instability happening between two miscible fluids in a porous domain brings advantages in various areas, comprising of chemical and petroleum engineering, environmental engineering, and medicine. Viscous fingering (or Saffman-Taylor) instability (VFI) arises when a low-viscosity fluid is injected to displace a high-viscosity one. From a fluid dynamics point of view, the invading fluid with higher mobility (lower viscosity) penetrates the displaced fluid resulting in appearance of fingers at the interface. In oil recovery, these fingers reduce efficiency of the oil displacement and pose an economic threat for oil and gas industries. So, scrutinizing the physical parameters impacting the instability is crucial. One of the ubiquitous assumptions considered in the numerical studies of VFI is the Boussinesq approximation. This approximation ignores density variations except in the term multiplied by gravity (Buoyancy term). Although this assumption simplifies numerical as well as analytical solutions, it cannot provide precise information, notably when dealing with oil containing dissolved gas. In this study, we try to shed light on the effect of slight compressibility on VFI through the simulation of an iso-thermal miscible displacement flow in a horizontal rectangular homogeneous porous domain. Our simulation study is based on the finite difference method (FDM) with a semi-implicit time stepper. The pivotal

goals are to delineate, both qualitatively and quantitatively, whether the fluid's compressibility enhances or attenuates the instability. Thus the influence of fluid's compressibility on breakthrough time, sweep efficiency, mixing zone length, and flow structure are investigated. The results demonstrate that slightly compressible fluids have different fingering patterns compared to incompressible ones. The involved mechanisms retard the growth of the ramifications. This result is also confirmed by the quantitative analyses. In earlier times, the pressure gradient is partially absorbed by compression of the fluids and the mixing zone length (MZL) for slightly-compressible fluids is smaller than the incompressible flow's MZL in the diffusive dominated regime. This effect causes a delay in the starting of fingering dominated period as well which results in the increase of the breakthrough time that brings a rise in sweep efficiency. The outcome of this research is a good explanation for the discrepancy between the experimental and numerical results of previous works.

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MS14 / 591

## A parallel recursive implementation of the Multiscale Perturbation Method for two-phase flow

**Authors:** Arthur Espírito Santo<sup>1</sup> ; Eduardo Abreu<sup>2</sup> ; Felipe Pereira<sup>3</sup> ; Fabricio Sousa<sup>4</sup> ; Franciane Rocha<sup>4</sup>

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We investigate the approximation of two phase flows in porous media using the Multiscale Perturbation Method (MPM) [1] to compute velocity fields, in a parallel recursive implementation. Since an elliptical equation must be solved at each simulation level in multiphase flow problems approximated by operator splitting, the MPM makes use of classical perturbation theory in order to avoid all multiscale basis functions to be recomputed. We replace the full upgrade of local solutions with the reuse of multiscale basis functions that have previously been calculated by making use of the Recursive Multiscale Robin Coupled Method [2], developed in a multiscale parallel domain decomposition framework. It is well known that non-overlapping domain decomposition schemes have great potential to take advantage of multi-core, state-of-the-art parallel computers, and the current approach is capable of speeding up the solution of multiphase flow problems. Avoiding the recalculation of basis functions is a prominent feature that can be extended to situations in which countless problems with relatively close permeability fields must be solved, such as uncertainty quantification problems. Here, we present numerical examples for challenging, high-contrast permeability fields and investigate the good scalability properties of MCRM for large problems in subsurface flows.

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MS9 / 708

## A parallelized method to model combined conductive-radiative heat transfer at local scale within highly porous media

**Authors:** Atin Kumar<sup>None</sup>; Jerome Vicente<sup>None</sup>; Yann Favennec<sup>None</sup>; Benoit Rousseau<sup>None</sup>

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In the field of high temperature applications such as energy conversion processes based on concentrated solar heating or the design of thermal protection systems for space vehicles, porous materials with high porosity (75-95 %) know today a growing interest. Two categories of porous materials which can be commonly described by an interconnected network of solid constituents surrounded by a fluid phase are thus investigated: cellular materials and fibrous materials. Indeed, they globally exhibit a high strength-to-weight ratio, a high volumetric surface, a good flow-mixing capability with other interesting properties. The solid network confers to these materials, a complex texture from which the intimate link between its main textural descriptors and its physical properties still remains unclear and impede their industrial uses.

This latter statement is particularly true for the effective thermal conductivity (ETC), especially when temperatures becomes high ( $T > 1000^\circ\text{C}$ ). The ETC depends on conduction and radiation heat transfers occurring simultaneously within the volume of the porous medium [1]. To get a better understanding on this quantity, a parallelized numerical solver based on domain decomposition applied to a 3D voxelized image where the whole physics is portrayed, is developed. This discrete scale approach which requires a prior and accurate knowledge of local thermal properties of constituents (thermal conductivity and optical properties) constitutes an alternative solution to those based on the continuous scale approach which requires the prior and exact knowledge of the effective thermal properties [2] (effective solid thermal conductivity, effective extinction coefficient, albedo and scattering phase function). Once the 3D image is described and analysed using the free morphology analysis software iMorph, a subdivision of the numerical domain is performed to provide suitable subdomains in which conjugated heat transfers are computed. The dimensions of the subdomains are selected to respect the underlying physics. Then, a Finite Volume Method is applied to solve the conductive transfers for the associated set of voxels within a subdomain, and an accelerated ray tracing method is applied to treat the radiative heat transfers between subdomains. This strategy allows to gain the computational time without compromising with the accuracy of the global solution. After validating the new code on academic 3D porous geometries for which the thermal behaviours at high temperatures had been previously computed [3], ETC computations are carried out on cellular samples, and the results obtained by varying the contribution of conduction and radiation on effective heat transfer i.e., by varying the Stark number [3] will be presented during the communication and discussed.

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[2] Leroy V, Goyeau B, Taine J. Coupled Upscaling Approaches For Conduction, Convection, and Radiation in Porous Media: Theoretical Developments. *Transport in Porous Media*. 2013;98:323-47.

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MS24 / 253

## **A phase-field method for propagating fluid-filled fractures coupled to a surrounding porous medium**

**Authors:** Thomas Wick<sup>1</sup> ; Sanghyun Lee<sup>2</sup> ; Mary Wheeler<sup>3</sup>

<sup>1</sup> *Leibniz University Hannover*

<sup>2</sup> *Florida State University*

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In this presentation, we revisit our efforts to model fluid-filled fracture propagation in a porous medium. Several challenges and extensions in mathematical modelling as well as the design of numerical methods will be discussed. Along with these theoretical and algorithmic accomplishments, a computational framework IPACS has been developed, which is substantiated with some numerical simulations.

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MS1 / 681

## **A physics-based model to predict the impact of horizontal layers on CO<sub>2</sub> plume migration**

**Author:** Maartje Boon<sup>1</sup>

**Co-author:** Sally M. Benson<sup>1</sup>

<sup>1</sup> *Stanford University*

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Geologic carbon sequestration can play an important role in reducing the amount of greenhouse gasses emitted to the atmosphere. To ensure the long-term security of the injected CO<sub>2</sub>, a good understanding of the fate of the plume is needed. Small scale (mm-m scale) rock structure heterogeneities impact the local capillary forces and, therefore, a capillary potential at the scale of the heterogeneity can exist. This can result in capillary induced flows and trapping and can have significant impact on the migration of the injected CO<sub>2</sub>. As a result the lateral migration of the CO<sub>2</sub> plume is often not well predicted by reservoir simulators where small-scale rock heterogeneity is not taken into account. Small-scale rock heterogeneity can be incorporated into larger scale models by using upscaled effective multi-phase flow parameters. These effective parameters are flow-rate dependent due to the dependence of the saturation distribution on the viscous-capillary force balance. We present a new physics-based model that can obtain effective flow-rate dependent relative permeability and capillary pressure functions in horizontally layered systems over the full velocity range, analytically (Figure 1). For this purpose a new capillary number, RVC, has been derived that correctly captures the viscous-capillary force balance for horizontally layered systems. The model



is based on the fractional flow approach and the obtained effective flow-rate dependent fractional flow functions can be implemented into an extended radial Buckley-Leverett solution to look at the impact of mm-m scale heterogeneity on the frontal advance of the CO<sub>2</sub> plume (Figure 2). The local RVC in the case of radial Buckley-Leverett systems is a function of two competing factors, the fractional flow of CO<sub>2</sub> and flow-rate. Both factors decrease with radial distance, and the fractional flow of CO<sub>2</sub> increases with time. A decrease in the fractional flow of CO<sub>2</sub> moves the system towards the VL, while a decrease in flow-rate moves the system towards the CL. The counterbalance between those two factors determines, together with the absolute permeability, the permeability ratio, and aspect ratio of the layers, when and where the VL to CL transition occurs. When the system transitions from the VL to the CL the relative permeability of the CO<sub>2</sub> phase increases, while the relative permeability of the water phase decreases. As a result, the CO<sub>2</sub> plume travels further when the system moves towards the CL. Our work shows that for injection rates and volumes commonly used at injection sites, the CL is reached quickly suggesting that flow-rate dependency is only important during the initial phase of the injection period. If the objective is the prediction of the lateral extent of the plume at the end of the injection period, the use of CL saturation functions will be valid, even close to the injection well.

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MS6-A / 435

## A pore-network upscaling framework for the nanoconfined thermodynamic phase behavior in shale rocks

**Authors:** Sidian Chen<sup>1</sup> ; Jiamin Jiang<sup>2</sup> ; Bo Guo<sup>1</sup>

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Hydrocarbon recovery from unconventional shale formations has reshaped the global energy landscapes. The presence of extensive nanopores introduces unique thermodynamic fluid phase behaviors—owing to large pressure differentials across fluid-fluid interfaces and strong fluid-wall interactions. While the nanoconfined phase behavior has been extensively studied in a single nanopore or a few pores, its manifestation in complex nanopore networks remains poorly understood. Rigorously derived macroscopic phase behavior formulations are not yet available.

To address this knowledge gap, we develop a novel upscaling framework for deriving macroscopic phase behavior formulations in realistic nanopore networks (e.g., nanopore networks extracted from high-resolution digital images of shale samples). The framework employs a generalized phase equilibrium model that explicitly accounts for the impact of capillary pressure and multicomponent adsorption in each pore. Assuming thermodynamic equilibrium across the pore network, macroscopic phase behavior variables for the entire pore network are then derived by integrating the variables from the individual pores. This leads to a macroscopic network-scale phase equilibrium model that naturally accounts for the size- and geometry- dependent nanoconfinement effects of a complex pore structure. Simulated phase behaviors in multiscale pore networks that consist of millions of nanopores demonstrate that 1) the phase behavior in a pore network—controlled by the multiscale pore structure—significantly deviates from that in a single nanopore and 2) heavier components tend to reside in smaller pores driven by capillary trapping of the liquid phase and preferential adsorption. The upscaled phase behavior model shares the same mathematical structure as that of a standard phase behavior model and can be readily incorporated in commercial reservoir simulators.

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MS4 / 209

## A poro-elasto-visco-plastic model of the dewatering of a two-phase suspension

**Author:** Eaves Tom S.<sup>1</sup>

**Co-authors:** Paterson Daniel T.<sup>2</sup>; Hewitt Duncan R.<sup>3</sup>; Balmforth Neil J.<sup>2</sup>; Martinez D. Mark<sup>2</sup>

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A poro-elasto-visco-plastic model for the consolidation of a two-phase suspension is presented, motivated by the compaction and dewatering of wood-fibre pulp. For that material, traditional two-phase models of particulate porous media based upon plastic yielding of the particle network prove insufficient to capture the observed dynamics. The incorporation of viscous effects stemming from the compaction of the wood-fibre-network assists the model in reproducing experimental dewatering tests at moderate rates of compaction. However, during more rapid dewatering there is clear emergence of an elastic behaviour in the wood-fibre network. We present a poro-elasto-visco-plastic extension of the model, its calibration for wood-pulp using quasi-static cycles of loading and unloading, and demonstrate its improved representation of the rapid dewatering experiments.

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MS7 / 171

## A posteriori estimates for the Richards equation (nonlinearity, degeneracy & heterogeneity)

**Authors:** Koondanibha Mitra<sup>1</sup>; Martin Vohralik<sup>2</sup>

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Richards equation is commonly used to model the flow of water and air through soil, and it serves as a gateway equation for multiphase flow through porous domains. With pressure  $p$  being the primary variable, it equates

$$\begin{aligned} \partial_t S(p) - \nabla \cdot [\mathbf{K} \cdot \kappa(S(p)) \cdot \nabla p - \mathbf{g}] = f(\mathbf{x}, t), \end{aligned}$$

$\tag{1}$   
 $\end{align}$   
 where  $S : [-\infty, \infty] \rightarrow [0, 1]$  is the increasing saturation function,  $\kappa : [0, 1] \rightarrow [0, 1]$  is the relative permeability function,  $\mathbf{K}$  the absolute permeability tensor,  $\mathbf{g}$  the gravitational acceleration, and  $f$  the reaction/absorption term. Apart from having nonlinear advection/reaction/diffusion components, Richards equation also exhibits both parabolic-hyperbolic (at  $S(p) = 0$  since  $\kappa(S(p)) = 0$ ) and parabolic-elliptic (at  $S(p) = 1$  since  $S'(p) = 0$ ) type of degeneracies. Further challenges in its numerical treatment comes from the heterogeneity in  $\mathbf{K}$ .

In this study, we provide fully computable, locally space-time efficient, and reliable a posteriori error bounds [1] for numerical solutions of the fully degenerate Richards equation: if  $p$  is the exact solution of (1) and  $p_{h\tau}$  is a known approximate solution, then for a composite distance metric  $\text{dist}(\cdot, \cdot)$  it holds that

$$\underline{\eta}(p_{h\tau}) \leq \text{dist}(p, p_{h\tau}) \leq \bar{\eta}(p_{h\tau}), \tag{2}$$

$\end{align}$   
 where both  $\underline{\eta}(\cdot)$  and  $\bar{\eta}(\cdot)$  are fully computable, and a version of the lower bound holds in any space-time subdomain. The bounds are proven in a variation of the  $H^1(H^{-1}) \cap L^2(L^2) \cap L^2(H^1)$  norm which corresponds to the minimum regularity inherited by the exact solutions, thus avoiding further smoothness assumptions like in [2]. For showing the upper bound, error estimates are derived individually for the  $H^1(H^{-1})$ ,  $L^2(L^2)$  and the  $L^2(H^1)$  error components with a maximum principle and a novel degeneracy estimator being used for the last one. Local and global space-time efficient error bounds are obtained following [3]. Error contributors such as flux and time non-conformity, quadrature, linearisation, data oscillation are identified and separated. The estimates also work in a fully adaptive space-time discretization and linearisation setting.

To investigate the effectiveness of the estimators, numerical tests are conducted for non-degenerate and degenerate cases having exact solutions. It is shown that the estimators correctly identify the errors, both spatially and temporally, up to a factor in the order of unity. Finally, to demonstrate the prowess of the estimators, a degenerate problem is analyzed in a heterogeneous, anisotropic domain with discontinuous initial condition and mixed boundary conditions.

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## A quantitative study of transition states between single-phase steady flows in a microfluidic device

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Velocity fields in flow in permeable media are of great importance to many subsurface processes such as geologic storage of CO<sub>2</sub>, oil and gas extraction, and geothermal systems. Steady-state flow is characterized by velocity fields that do not change significantly over time. The flow field transitions to a new steady state once it experiences a disturbance such as a change in flow rate or in pressure gradient. This transition is often assumed to be instantaneous, which justifies expressing constitutive relations as functions of instantaneous phase saturations. In this work, we examine the evolution of velocity fields in a surrogate quasi-2D permeable medium using a microfluidic device and a high-speed camera. Tracer particles, i.e., microspheres with a diameter of one micrometer, are injected into the medium along with DI water. The evolution of the velocity field is examined by tracing these particles in the captured images using a multi-pass particle image velocimetry algorithm. The results suggest that transition period between steady-states for an incompressible fluid takes a finite and non-negligible amount of time. Finally, we examine the impact of the magnitude of the change in the pressure gradient on this transition period.

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## **A review on the use of microbial induced calcite precipitation for problematic soil engineering**

**Author:** Ehsan Nikoee<sup>1</sup>

**Co-author:** Ghassem Habibagahi<sup>1</sup>

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The use of conventional techniques for soil stabilization often involves chemical compounds which are not environmentally friendly and can be hazardous. Moreover, newly introduced regulations which target zero CO<sub>2</sub> emission demand new construction policies and alternative construction solutions. When it comes to soil improvement, reducing the level of greenhouse gas emission would mean searching for eco-friendly stabilizing agents rather than resorting to traditional ones such as lime and cement. Biological soil stabilization techniques which include the use of a variety of microorganisms such as bacillus, cyanobacteria, microalgae [e.g.,1-6], and/or the use of enzymes present in the microbial metabolic paths [e.g., 7], as well as biopolymers [e.g., 8-9] are among alternative solutions for soil improvement. In this contribution, a review on different biological soil stabilization techniques will be presented. The aim is to characterize different biological techniques and their strength and challenges. Then the focus is placed on the class of methods which is based on the microbial calcite precipitation (MICP) and its use for problematic soil engineering. The application of MICP for problematic soil engineering will be reviewed and the recent findings on the efficiency and efficacy of MICP to treat dispersive, expansive and collapsible soils [10-14] are briefly explained and suggestions for future studies, on this topic, are put forward.

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MS20 / 343

## A sequential grid-block upscaling method for highly heterogeneous tumors: application to osteosarcoma

**Authors:** Adel Moreno<sup>1</sup> ; Michel Quintard<sup>1</sup> ; Anthony Mancini<sup>2</sup> ; Anne Gomez-Brouchet<sup>3</sup> ; Pacal Swider<sup>None</sup> ; Pauline Assemat<sup>4</sup>

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Osteosarcoma is a primary bone tumour that occurs mainly in adolescents and young adults. The survival rate at 5 years is 70% and drops to 25% for patients with metastases or poor responders to treatment [1]. Therapeutic strategies have not evolved for more than three decades and new developments are needed to improve the specific management of patients.

Like the majority of complex genomic sarcomas, this type of tumours presents strong spatial heterogeneities. In the case of osteosarcoma, there are heterogeneities in bone micro-architecture, cell density but also in the response to treatment due to the potentially localised effect of chemotherapy [2]. Because of the cell populations involved in the evolution of osteosarcomas such as osteoblasts, osteoclasts or osteocytes, it is supposed that osteosarcoma is highly sensitive to the mechanical effects occurring at various spatial scales [3].

At the tissue scale, the osteosarcoma can be considered as porous medium involving various phases (bone, fluid and cells). It is admitted that transport mechanisms and structural deformations play a fundamental role in disease evolution but also on treatment efficiency. Therefore, it is important to determine accurately bone mechanical properties.

The aim of this work is to study different transport mechanisms (interstitial flow, diffusion), structural mechanics (linear elasticity) and poromechanics in the porous tumour at the tissue scale by an approach based on upscaling methods. This methodology rely on histological and immunohistological binarized sections of surgical specimens from a Toulouse patients cohort (CRB Cancer Toulouse). The statistical study of the osteosarcoma micro-architecture shows that the identification of characteristic lengths is complex and that a separation of spatial scales is not necessarily identified. To solve this problem, a sequential grid-block upscaling approach was therefore chosen [4].

We propose to study the 2-step sequential Grid-Block method for each physical mechanism mentioned above. In order to reduce the influence of boundary conditions on the sequential process, an extend-local method has been developed for the first upscaling. These methods have been implemented with the finite element toolbox FEniCS [5]. The dependence to the various methods parameters (boundary conditions, Grid-Block size etc) of the resulting tensors and their properties were studied.

Through this approach, mechanical properties and biological parameters (e.g. cell population density) can be correlated. It is then possible to obtain new quantitative mecano-biological information on bone tumours from patients follow-up images and potentially to obtain markers useful in patient-specific treatment management.

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MS14 / 689

## A sequential implicit solver for two-phase subsurface flows using the Multiscale Robin Coupled Method

**Author:** Franciane Rocha<sup>1</sup>

**Co-authors:** Fabricio Sousa<sup>1</sup>; Roberto Ausas<sup>1</sup>; Gustavo Buscaglia<sup>1</sup>; Felipe Pereira<sup>2</sup>

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Multiscale domain decomposition methods are a suitable choice when dealing with huge meshes arising from the discretization of the equations modeling multiphase flows in reservoir simulations. They allow the global solution to be computed in coarse meshes, while detailed basis functions are produced locally (usually in parallel) in a much finer grid. We are concerned with the solution of non-linear two-phase flow models using the recently developed Multiscale Robin Coupled Method (MRCM, [1]). This method allows for great flexibility on the choice of interface spaces that couple local solutions, with a clear advantage in highly heterogeneous porous media when compared to some standard multiscale mixed methods. In the presence of strong heterogeneities, it is well known that explicit schemes for the transport of saturation suffer from severe time-step restrictions. Therefore we investigate the combination of the MRCM with implicit transport schemes, allowing for the use of large time steps when compared to explicit time integration approaches. A sequential implicit strategy is proposed, with different trust-region algorithms to ensure the convergence of the transport solver. Improvement in the accuracy of the MRCM is investigated, considering alternative choices for the interface spaces other than the classical polynomials, since they are not optimal for high-contrast channelized permeability fields. Our numerical results have shown that the proposed method yields accurate and computationally efficient results for two-phase subsurface flows.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

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MS7 / 706

## A space-time multiscale mortar mixed finite element method for flow in porous media

**Authors:** Caroline Japhet<sup>1</sup> ; Manu Jayadharan<sup>2</sup> ; Michel Kern<sup>3</sup> ; Martin Vohralik<sup>4</sup> ; Ivan Yotov<sup>2</sup>

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We develop a space-time mortar mixed finite element method for parabolic problems modeling flow in porous media. The domain is decomposed into union of subdomains with non-matching grids and different time steps. The space-time variational formulation couples mixed finite elements in space with discontinuous Galerkin in time. Continuity of flux across space-time interfaces is imposed via coarse-scale space-time mortar finite elements, resulting in correct mass conservation. A priori error estimates for the spatial and temporal error are established. A space-time non-overlapping domain decomposition method is developed that reduced the global problem to a space-time coarse-scale mortar interface problem. Each interface iteration requires solving space-time subdomain problems, which is done in parallel. The convergence of the interface iteration is analyzed. Numerical results illustrate the theoretical results and the flexibility of the method for modeling flow in heterogeneous porous media with features localized in space and time.

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## A stochastic analysis of the non-Newtonian hydraulic behavior of rough fractures

**Authors:** Alessandro Lenci<sup>1</sup> ; Yves Méheust<sup>2</sup> ; Mario Putti<sup>3</sup> ; Vittorio Di Federico<sup>4</sup>

<sup>1</sup> *Università di Bologna Alma Mater Studiorum*

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Fluids involved in activities occurring in fractured underground reservoirs, either related to natural resource recovery (e.g., hydrofracturing, drilling, geothermal exploitation) or environmental remediation schemes, often exhibit complex rheology. The micro-structure of foams, muds, emulsions, or colloidal suspensions induces shear-thinning in the continuum scale mechanical behaviour, which can be described by the Ellis rheology. This three-parameter model has a Newtonian low-shear rate behaviour of apparent viscosity  $\eta_0$ , a high-shear rate power-law trend with exponent  $n$ , and a transition between the two regulated by a characteristic stress  $\tau_{1/2}$ . Such fluids often flow in rock fractures having rough walls characterized by long-scale correlations in the topography, i.e., a self-affine scale invariance at all scales. The facing walls of a given fracture are also mated at scales larger than a

characteristic correlation length scale. Such geometries can be reproduced numerically utilizing an FFT-based algorithm. The fracture closure is then measured as the ratio of the aperture field's roughness amplitude to the mean fracture aperture. The investigation of the non-Newtonian hydraulic behaviour of such natural or artificial fractures implies a considerable mathematical and numerical effort to properly account for non-linearities and medium geometry. A full stochastic analysis of large fractures with a variety of statistical descriptive parameters via Monte Carlo simulations is almost prohibitive considering a fully 3-D simulation of the flow. The flow of a shear-thinning fluid through a variable aperture fracture can instead be described under the assumptions of the lubrication theory, a depth-averaged formalism that reduces the model formulation to a single two-dimensional non-linear PDE. A numerical code has been implemented adopting the finite volume method, with the fracture discretized on a staggered grid, defining the pressures at the centre of each finite volume and the aperture at each side. The system of non-linear equation is solved adopting the Newton-Krylov method, considering a continuation strategy to face strong non-linear cases (very low  $n$  values), and solving the linearized symmetric system of equations via variable-fill-in incomplete Cholesky preconditioned conjugate gradient algorithm. A Monte Carlo framework is adopted to study the influence of rheology, fracture dimension and pressure gradient on fracture hydraulic behaviour, generating  $NMC = 1000$  realizations of the aperture field. The approach allows characterizing the hydraulic behaviour via ensemble statistics, such as the PDFs of the velocity fields and the dependence of the fracture transmissivity on fracture closure, and how it is impacted by the fluid's shear thinning behaviour. Fracture flow is mainly cocurrent, presenting narrow PDFs with nearly exponential decay. Evident channelling and localization effects are associated with strongly heterogeneous aperture fields and very shear-thinning fluids. In these cases, the probability distributions of velocity components PDFs show wide tails deviating from the exponential decay, and the fracture transmissivity is much higher compared with the Newtonian case of identical mean aperture.

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MS21 / 5

## **A theoretical analysis of the nonlinear behaviors in the measurements for two-phase flow in low-permeability core considering the capillary effects**

**Authors:** Xiao-Hong Wang<sup>1</sup> ; Yu-Min Yao<sup>1</sup> ; Min Wang<sup>1</sup> ; Zhi-Feng Liu<sup>1</sup>

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In recent years, the flow behaviors in low-permeability media have received much attention. Some experimental measurements indicate that single-phase flow in the low-permeability core seems to present the nonlinear behaviors rather than obeying the Darcy's law. However, there are different opinions on the explanation of the experimental measurements. For two-phase flow, some scholars pointed out that the capillary pressure (Jamin effect) is can cause the nonlinear seepage behavior. However, there is no corresponding mathematical model to describe it.

When two-phase fluid flows into the non-capillary force container from the core sample containing capillary force, the phase saturations at the outlet end of the core increase significantly compared with the rest of the area. This phenomenon was called as the capillary end effect. Considering capillary end effect, Yao et al. proposed a two-phase flow well model for low permeability gas reservoirs considering capillary end effect.

Considering the strong capillary pressure contrast between matrix and fracture in low-permeability reservoirs, Wang et.al pointed out that, there are three flow patterns for the two-phase flow across



the matrix-fracture interface: (1) When the pressure difference between matrix and fracture can overcome the capillary end effect, both two-phase fluids flow from matrix to fracture and saturation gradient and the non-wetting phase pressure gradient diverged near the matrix interface; (2) When the pressure difference between matrix and fracture cannot overcome the capillary end effect, only non-wetting phase flows from matrix to fracture; (3) Both two phases flow from fracture to matrix, wetting phase pressure is discontinuous across matrix - fracture interface.

In this article, the two-phase flow behaviors in the low-permeability core experiment are analyzed. The dramatic capillary pressure difference between the core and the vessel will lead to wetting phase pressure discontinuity at the core inlet and the divergence of saturation gradient and non-wetting phase pressure gradient at the core outlet. Under the condition of that the two-phase flow in the low-permeability core satisfies the generalized Darcy's law, a rigorous mathematical analysis is presented that the dramatic capillary pressure difference between the core and the vessel can cause the pressure difference-flow rate curve to be nonlinear.

Low permeability reservoirs are usually highly heterogeneous and there are many natural fractures in the reservoirs. The multi-scale effects of flow on the matrix-natural fracture interface result in strong capillary heterogeneity. So even though the flow in the matrix and natural fractures satisfies the generalized Darcy law, the two-phase flow in low-permeability reservoirs may show the nonlinear behaviors at macroscopic reservoirs scales.

Capillary end effect can cause great error to the steady-state relative permeability measurement experiment data. Through numerical simulation, Gupta et al. (2016) proposed an intercept method to correct the steady-state relative permeability measurement data considering capillary end effect. Andersen et al. (2020) gave a mathematical proof of Gupta et al.'s intercept method in the condition of the specific capillary and relative permeability curves. In this article, a rigorous mathematical proof of this method is proposed.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS6-A / 168

## ANALYTICAL SOLUTION FOR THE POPULATION-BALANCE MODEL DESCRIBING FOAM

**Authors:** Rosmery Q. Zavala<sup>1</sup> ; Luis F. Lozano<sup>1</sup> ; Pacelli Zitha<sup>2</sup> ; Grigori Chapiro<sup>3</sup>

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Recently a simple but robust model was proposed for describing foam flow in porous media. Numerical solutions to this model were found to be in good agreement with CT scanned nitrogen foam flow experiments in Bethheimer sandstone cores, where the foam was stabilized by Alpha Olefin Sulfonate (AOS) surfactant, Simjoo and Zitha 2015. Here, we present analytical solutions for a further simplified version of this population balance foam model. We investigate and classify possible solutions for different injection conditions and varying kinetic foam generation and coalescence parameters, see Lozano et al. 2021. We found that the analytical solutions' behavior changes at the transition between two regions, similar to rarefaction/shock solutions for the Buckley-Leverett equation. Region I presents a traveling wave solution in a good match with two different sets of experimental data. In this region, the analytical solutions also match the original model's numerical simulations. Region II corresponds to solutions as a sequence of waves: one spreading wave and one traveling wave pointing out to flow profiles different from those found in the experiments.

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MS15 / 161

## Accelerating Micro-Macro Models for Two-Mineral Reactive Systems with Machine Learning

**Author:** Stephan Gärttner<sup>1</sup>

**Co-authors:** Peter Frolkovic<sup>2</sup>; Peter Knabner<sup>3</sup>; Nadja Ray<sup>4</sup>

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In this talk, we present an effective micro-macro model for reactive flow and transport in evolving porous media exhibiting two competing mineral phases. As such, our approach comprises flow and transport equations on the macroscopic scale including effective hydrodynamic parameters calculated from representative unit cells. Conversely, the macroscopic solutes' concentrations alter the unit cells' geometrical structure by triggering dissolution or precipitation processes on the distinct mineral surfaces. Gradually, such processes result in complex and hardly predictable geometries. Therefore, these do not allow for low dimensional parameter representations. Accordingly, associate effective parameters cannot be covered by simple heuristic laws. Hence, we derive hydrological parameters directly from the full geometry represented by level-set methods.

The numerical realization of such micro-macro models poses several challenges, especially in terms of computational complexity due to the increased dimensionality of the problem. Costly computations of effective parameters directly from the representative geometry often constitute a bottleneck in the simulation of highly heterogeneous media. In this talk, the significant performance enhancements arising from machine learning techniques are evaluated. To this end, convolutional neural networks (CNNs) are trained on geometries derived from geological microCT scans to predict hydrodynamic parameters such as permeability and diffusivity. The pretrained networks are subsequently

deployed in a micro-macro simulation. We investigated the results in terms of computation time reduction and maintenance of high predictive quality.

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MS25 / 766

## Accurate determination of the time-validity of Philip's two-term infiltration equation

**Author:** Jasper Vrugt<sup>1</sup>

**Co-author:** Parakh Jaiswal<sup>1</sup>

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Many different equations have been proposed to describe quantitatively the infiltration process. These equations range from simple empirical equations to more advanced deterministic model formulations of the infiltration process and semi-analytical solutions of Richards' equation. The unknown coefficients in these infiltration functions signify hydraulic properties and must be estimated from measured cumulative infiltration data,  $\tilde{I}(\tilde{t})$ , using curve fitting techniques. From all available infiltration functions, the two-term equation,  $I(t) = S\sqrt{t} + cK_s t$  of Philip (1957) has found most widespread application and use. This popularity has not only been cultivated by detailed physical and mathematical analysis, the two-term infiltration equation is also easy to implement and admits a closed-form solution for the soil sorptivity,  $S$  ( $L/T^{1/2}$ ), and multiple,  $c$  (-), of the saturated hydraulic conductivity,  $K_s$  ( $L/T$ ). Yet, Philip's two-term infiltration function has a limited time validity,  $t_{\text{valid}}$  ( $T$ ), and consequently, the use of measured cumulative infiltration data,  $\tilde{I}(\tilde{t})$ , beyond  $t = t_{\text{valid}}$  will corrupt the estimates of  $S$  and  $K_s$ . Philip (1957) provides theoretical guidelines on the time validity, yet, these estimates need to be corroborated experimentally. In this paper, we introduce a new method to determine simultaneously the values of the coefficient  $c$ , hydraulic parameters,  $S$  and  $K_s$ , and time validity,  $t_{\text{valid}}$ , of Philip's two-term infiltration equation. Our method is comprised of two main steps. First, we determine independently the soil sorptivity,  $S$ , and saturated hydraulic conductivity,  $K_s$  by fitting the implicit infiltration equation of Haverkamp et al. (1994) to measured cumulative infiltration data using Bayesian inference with DREAM Package of Vrugt (2016). This step is made possible through a novel, exact and robust numerical solution of Haverkamp's infiltration equation, and returns as byproduct the marginal distribution of the parameter  $\beta$ . In the second step, the maximum likelihood values of  $S$  and  $K_s$  are used in Philip's two-term infiltration equation, and used to determine the optimal values of  $c$  and  $t_{\text{valid}}$  via model selection using the Bayesian information criterion. To benchmark, test and evaluate our approach we use cumulative infiltration data simulated by HYDRUS-1D for twelve different USDA soil types with contrasting textures. This allows us to determine whether our procedure is unbiased as the inferred  $S$  and  $K_s$  of the synthetic data are known before hand. Results demonstrate that the estimated values of  $S$  and  $K_s$  are in excellent agreement with their "true" values used to create the infiltration data. Furthermore, our estimates of  $c$ ,  $\beta$  and  $t_{\text{valid}}$  depend strongly on texture and fall within the ranges reported in the literature. Our findings are corroborated by analysis of real-world data. Our study addresses four areas of active research by Prof. Vereecken, namely (1) measurement and modeling of water infiltration into variably-saturated soils, (2) development of numerical methods for subsurface flow and transport, (3) soil moisture measurement and characterization and (4) inverse methods and uncertainty quantification. As I have known Harry for about 15 years and visited him on several occasions, I'd be remiss if I did not share a few personal anecdotes about him (time permitting).

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

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## Accurate numerical simulation of electrodiffusion and water movement in brain tissue with cortical spreading depression as a case study

**Author:** Ada Johanne Ellingsrud<sup>1</sup>

**Co-authors:** Marie Elisabeth Rognes ; Patrick Farrell ; Nicolas Boule ; Didrik Dukefoss ; Rune Enger ; Klas Pettersen ; Geir Halnes

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Mathematical modelling of ionic electrodiffusion and water movement is emerging as a powerful avenue of investigation to provide new physiological insight into brain homeostasis. However, in order to provide solid answers and resolve controversies, the accuracy and precision of the predictions are essential. Here, we consider an homogenized model for ionic electrodiffusion and osmosis comprising a non-trivial system of non-linear and highly coupled partial and ordinary differential equations that govern phenomena on disparate time scales. We study numerical challenges related to approximating the system and validate the model against values from experimental studies in the physiologically relevant setting of cortical spreading depression (CSD). CSD is a wave of electrophysiological hyperactivity accompanied by substantial shifts in ionic concentrations and cellular swelling. We evaluate different associated finite element-based splitting schemes in terms of their numerical properties, and find that the schemes display optimal convergence rates in space for problems with smooth manufactured solutions. However, the physiological CSD setting is challenging: we find that the accurate computation of CSD wave characteristics (wave speed and wave width) requires a very fine spatial and fine temporal resolution. Further, the data for several CSD hallmarks obtained computationally, including wave propagation speed, direct current shift duration, peak in extracellular potassium concentration as well as a pronounced shrinkage of extracellular space, are well in line with what has previously been observed experimentally. Finally, we note that the model considered within this work may be applied to study a wide array of phenomena in brain physiology and pathology.

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## Adaptive Virtual Element Methods for simulations in Discrete Fracture Matrix models

**Author:** Andrea Borio<sup>1</sup>

**Co-authors:** Stefano Berrone<sup>2</sup>; Stefano Scialò<sup>1</sup>; Alessandra D'Auria<sup>1</sup>; Fabio Vicini<sup>1</sup>

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The simulation of flow and transport in poro-fractured media is a complex task, in particular from the point of view of mesh generation. Indeed, constructing good quality meshes that are conforming to the fractures internal to a rock matrix can be computationally expensive when the mesh has to be simplicial, as for standard Finite Element Methods.

In this talk we introduce novel strategies based on Virtual Element Methods (VEM) to perform simulations of flows in Discrete Fracture Matrix models. The flexibility of generalized polygonal meshes that can be handled by VEM, even allowing aligned edges and aligned faces, is a very useful tool for mesh generation. The presented strategies rely on the fast generation of polytopal meshes and on suitable refinement techniques designed for generalized polytopal meshes, that are used to adapt the mesh according to a posteriori error estimates, in order to reduce the number of degrees of freedom used to obtain high quality solutions.

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Stefano Berrone, Andrea Borio, Alessandro D'Auria, Refinement strategies for polygonal meshes applied to adaptive VEM discretization, *Finite Elements in Analysis and Design*, Volume 186, 2021, 103502, ISSN 0168-874X, doi:10.1016/j.finel.2020.103502. (<https://www.sciencedirect.com/science/article/pii/S0168874X20301827>)

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## Adaptive phase recovery method for three-dimensional porous media reconstruction from its bi-dimensional thin-section

**Authors:** Aleksei Cherkasov<sup>1</sup>; Andrey Ananav<sup>1</sup>; Aleksey Khlyupin<sup>1</sup>; Kirill Gerke<sup>None</sup>

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Determining the macroscopic properties of heterogeneous materials requires detailed knowledge of their porous structure. The most widely used experimental methods allow obtaining high-quality bi-dimensional images of porous media samples. At the same time, direct investigation of three-dimensional samples is a technologically complicated process and requires expensive laboratory equipment. Different approaches as simulated annealing [1, 2], truncated Gaussian random fields [3], multi-point statistics [4] are applied for the solution of this problem. These methods have such disadvantages as significant computing requirements and simplified representation of porous media. Authors [5] present a method for reconstruction of multiphase structure from two orthogonal thin sections based on the phase recovery algorithm. This method is conveys microstructure morphology of porous media but its performance leads to artifacts that can influence the macroscopic properties of a reconstructed sample.

The artifacts influence the permeability of the reconstructed sample because of the additional solid phase inside the pore space. To solve this problem, we offer another phase-recovery-based method. The main idea of the method is to approximate three-dimensional autoconvolution by the rotation of an input image bidimensional autoconvolution. We use adaptive spatial frequency filtering and dynamic correction in Fourier space to remove artifacts and improve the quality of reconstruction. The resulting method is highly efficient and allows us to obtain detailed reconstructions. We reconstruct samples of carbonate, sandstone, and ceramics from the thin-sections of microCT images (as it is shown in the figure) and compare permeabilities computed by finite differences method Stokes solver (FDMSS) [7] for originals and reconstructions. The reconstructed samples' capacity-volumetric properties show good compliance with the original samples.

**Time Block Preference:**

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## Additive Manufacturing Via Digital Light Processing of Durable Ceramic Porous Structures for Application to Combustion Systems

**Authors:** Giancarlo D’Orazio<sup>1</sup> ; Sadaf Sobhani<sup>1</sup>

<sup>1</sup> Cornell University

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Combustion in porous media leverages heat transfer between the reacting gas and the solid structure to enable enhanced combustion properties. By internally recirculating heat released from the combustion products upstream to the reactants via an inert solid matrix, porous media burners (PMBs) enable the reliable utilization of lean fuel/air mixtures and reduce pollutant emissions. The local porous structure of PMBs directly affects the total heat transfer across a porous material. However, conventional fabrication methods for the ceramic structures applied in PMBs produce locally random pore geometries and sizes within a range of global parameters. In this research, we demonstrate fabrication of porous ceramics with predefined and reproduceable microstructures to enable tailored PMBs.

The computational geometries of the porous structures are first carefully architected for fine control of the burner performance, then additively manufactured using digital light processing. These printed structures are then integrated in PMBs for testing where the thermal and mechanical properties of the structures as well as burner performance are characterized. Thermal cycling and shock are limiting factors for the lifespan of additively manufactured ceramic PMBs; to address this, triply periodic minimal surface (TPMS) structures make up the porous media, minimizing stress concentrations compared to foam based porous media and beam-based lattices. The thermal shock performance and thermal conductivity of various ceramic TPMS structures and slurry compositions is quantified. Further structural refinements to TPMS structures, such as tailored cell size and porosity grading, are incorporated into the design and fabrication of subsequent PMBs based on these characterizations.

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## **Additive Manufacturing of open porosities: from fabrication and characterization to the application**

**Author:** Robert Otto<sup>1</sup>

**Co-authors:** Christoph Kiener<sup>2</sup> ; Knut Sørby<sup>3</sup>

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Within the past years, Additive Manufacturing (AM) technologies could be established as a versatile complement to conventional means of manufacturing. Especially provided opportunities such as handling complex geometries and gaining control of various process parameters have become a driving force towards its use for industrial applications. Being data-based, AM technologies also allow a high degree of adaptability to customized designs. In this study, resulting novel possibilities for functionality driven designs will be investigated. Open porosities, structures that are known for being advantageous to heat transfer and flow applications, will be manufactured by Laser-Based Powder Bed Fusion (PBF-LB). The general concept of additively manufactured open porosities will be summarized. Further, the structures will be characterized by laboratory tests and simulations of their digital twin. Gained understanding will be utilized to correlate resulting functional properties to the manufacturing-input and thus to the design of future applications.

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MS7 / 170

## **Advancements in suction-induced fractures in multiphase porous media: Phase-field and data-driven multiscale modeling**

**Author:** Yousef Heider<sup>1</sup>

<sup>1</sup> *RWTH Aachen University*

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Whether naturally- or artificially-induced due to human activities, decreasing or increasing of suction in multiphase-fluid-saturated porous materials can lead to enormous changes in their thermo-hydraulic properties. In this, both the mathematical description and the numerical modeling of the coupled problem present a challenging task. The presentation considers the following two instances related to suction-induced fractures. (1) The drying-induced fracturing, which occurs due to increasing of the capillary pressure (air pressure minus water pressure) in low-permeable, unsaturated porous materials. (2) The micro-cryo-suction-induced fractures, which can be observed in saturated and unsaturated porous materials under freezing conditions.

In both cases, the macroscopic modeling of the induced fractures is based on continuum porous media mechanics extended by a diffusive phase-field fracture method. For the drying-induced fractures of unsaturated porous media, one has to deal with more than one pore fluid (e.g., water and air). In this case, the mechanical behavior can be expressed by using Bishop's effective stress principle, which considers the total stress, the capillary pressure, and saturation degree. For the micro-cryo-suction-induced fractures in saturated porous media, the water freezing is treated as a phase-change process. This is modeled using a different phase-field approach, in which the thermal energy derives the phase change and, thus, leads to occurrence of micro-cryo-suction due to the formation of the ice phase.

In addition to the continuum mechanical modeling and the conventional constitutive relations, machine learning (ML) presents a powerful tool in bridging the gap between the micro and the macro scales. In this, we employ self-designed/self-improved neural networks, which can be trained using datasets of microscale simulations, to produce constitutive relations for the macroscopic scale simulations. For instance, ML via deep recurrent neural networks (RNN) allows to generate of path-dependent retention curve models, which can capture the challenging hysteresis behavior. Numerical examples will be presented and include qualitative and quantitative comparisons with experimental data.

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## **An Assumed Enhanced Strain (AES) finite element approach in modeling fracture propagation in partially saturated porous media**

**Author:** Fushen Liu<sup>1</sup>

<sup>1</sup> *Zhejiang University*

**Corresponding Author:** fushenliu@zju.edu.cn

Fracture propagation in porous media is essential to many complex subsurface geoengineering systems, such as geological fault rupture, hydraulic fracturing, geothermal energy exploitation and waste water management and so on. Numerical methods have become more and more important in better understanding the coupled physics of those complex subsurface systems. In this work, an AES finite element approach is proposed to simulate fracture propagation in the partially saturated porous media. Compared with traditional finite element method, the AES approach allows the fracture to propagate inside the elements, does not require the element edges to be aligned with the fracture. Compared with the extended finite element method, the AES approach does not introduce new degrees of freedom into the global system of equations. The fractures in AES approach can be modeled locally at the Gauss point level and the explicit geometrical description of fractures can be avoided. The presentation will cover the formulation and some numerical aspects in implementing AES approach, and demonstrate its capability in simulating fracture propagation in the porous media with several numerical examples.

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MS7 / 415

## **An Efficient Solution Strategy for Variational Models of Brittle Fracture**

**Authors:** Erlend Storvik<sup>1</sup> ; Jakub Both<sup>1</sup> ; Juan Michael Sargado<sup>2</sup> ; Jan Martin Nordbotten<sup>1</sup> ; Florin Adrian Radu<sup>3</sup>

<sup>1</sup> *University of Bergen*

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There is an increasing interest in solvers for phase-field models of brittle fracture [2]. The governing equations for this problem originate from a constrained minimization of a non-convex

energy functional, and the most commonly used solver is a staggered scheme. This method shows robustness in comparison to the monolithic Newton method, however, the staggered scheme often requires many iterations to converge when fractures are evolving. The focus of our work is to accelerate the solver through a scheme that combines Anderson acceleration and over-relaxation. The method is applied as a post-processing technique, and therefore, already available software can be modified to include the acceleration method. Moreover, the activation of the scheme has a negligible cost. A numerical study, including well-known benchmark problems, that demonstrates the efficiency, and robustness of the method will be presented [1].

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## An adaptively coupled multiphysics model for compositional two-phase flow targeting underground gas storage

**Authors:** Beatrix Becker<sup>None</sup> ; Rainer Helmig<sup>1</sup> ; Bernd Flemisch<sup>1</sup>

<sup>1</sup> *University of Stuttgart*

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Compositional flow is an important feature of numerical models in the context of gas storage in the subsurface. In practice, not only maximum inflow and outflow rates, development of reservoir pressure and gas plume shape in time are important, but because the gas is to be extracted and, e.g., combusted in a turbine, its molecular composition is of great interest. In addition, dissolution of the storage gas into the brine phase reduces the total amount of retrievable and thus commercially usable gas. Due to uncertainties associated with geological data, efficient and accurate models for energy storage in the underground need to be developed, which is additionally challenging since modeling compositional effects generally increases the complexity of models and with that the computational cost. The concept of vertical equilibrium (VE) [1,2] can be exploited in the context of compositional flow to develop fast models that give accurate solutions. In addition to phase equilibrium, which develops when a less dense gas phase is injected into the resident brine and moves upward to pool below an impermeable barrier, chemical equilibrium forms along the vertical direction driven by the chemical potential between the phases and diffusion within the phases.

In this talk we present a vertically integrated compositional model which is adaptively coupled to a compositional full multidimensional model. We use the compositional VE model in regions of the domain where the compositional VE assumption is valid, and the compositional full multidimensional model everywhere else. We develop and analyze local criteria to identify where the compositional VE assumption is valid in the domain, including extraction and hysteretic effects on the coarse scale. During runtime of the multiphysics model, VE subdomains are identified by the local criterion and the models are assigned adaptively to those regions. We use two test cases:

gas injection into a horizontal layer and gas storage with reversed flow in an idealized dome-shaped aquifer, and show efficiency and accuracy of the compositional VE model and the compositional multiphysics model.

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MS6-B / 360

## An energy-preserving MAC numerical scheme for the Volume Of Fluid method and application on Taylor flows

**Authors:** Mohamed Id Moulay<sup>1</sup> ; Yohan Davit<sup>2</sup> ; Fabien Duval<sup>3</sup> ; Jean-Claude Latché<sup>3</sup> ; Michel Quintard<sup>2</sup>

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This work focuses on numerical simulations of two-phase flows in porous media at pore-scale in the framework of Volume Of Fluids (VOF) methods. The numerical scheme consists in solving on staggered grids the transport equation for the color function using an alternate directions algorithm together with the variable density incompressible Navier-Stokes equations using a pressure correction technique. A particular attention is paid to the discretization of the surface tension forcing term performed within the Continuum Surface Force formalism. Following the pioneering work of Jacqmin [1], we propose here an energy-conserving numerical scheme that consists in estimating the capillary force following a convex combination of the curvature with respect to the color function. The implementation is carried out in the CAFIF3S platform, a parallel open-source multiphase flow solver developed by IRSN and used for a wide range applications, including laminar or turbulent flows [2].

To validate our approach, we evaluate our results against several benchmark and test cases available in the literature. We first compare the energy-balanced discretization to the CSF Brackbill for a static bubble. An advanced comparison is carried out for the quantification of spurious currents using dimensionless velocity and vorticity for different Laplace numbers. We find that our scheme reduces spurious currents compared to CSF and generally performs well against other approaches that do not use a surface reconstruction (Abadie & al [3]). In a second step, we focus on the drainage of a liquid phase in a vertical cylindrical tube for a range of capillary numbers. We compare our results for film thickness against numerical approaches in the literature and the Bretherton model, as presented in Lasseux [4]. We find good agreement for several capillary numbers with Horgue & al [5], Lasseux [4] and the Bretherton model. We further discuss the robustness of our approach and general guidelines for optimizing mesh.

At last, we consider Taylor bubbles in a horizontal cylindrical tube, as presented in Gupta & al [6]. This type of flow is characterized by the presence of elongated bubbles, with diameters close to the width of the tube, that are separated by liquid plugs. The flow also features liquid films along the wall, which depend on the capillary number and can be extremely thin, thus posing a numerical challenge. A mesh convergence study is carried out for the calculation of film thicknesses. Our results are in good agreement with those of the benchmark. We also study of spurious currents at the interface as well as bubble shapes and gas hold-up.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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## **An investigation of drug release from granules linking structure, process and release performance**

**Author:** Faraj Shmam<sup>1</sup><sup>1</sup> *University of sheffield***Corresponding Author:** fashmam1@sheffield.ac.uk**Abstract**

An investigation of drug release from granules linking structure, process and release performance

Faraj Shmam, Rachel Smith, Kate Pitt

Particle Technology Group, Department of Chemical and Biological Engineering, The University of Sheffield, Mappin Street, Sheffield S1 3JD, UK

Granulation is a particle enlargement process where coarse or fine particles are agglomerated into large granules. These large granules are further processed to form tablets for oral solid dosage forms. In a high-shear granulation, the granule structure can be directly influenced by the granulation time and the amount of liquid binder added and this will have a strong influence on the dissolution rate of the granules. However, there is a lack of scientific understanding on the relationship between formulation, process and granule structure and performance. The aim of this work is to develop an experimental understanding of the relationship between granulation process parameters and granule structure and investigate the links between granule structure, granule dissolution and drug release profile.

In this study, microcrystalline cellulose was used as an excipient powder and polyethylene glycol as the binder. Acetyl salicylic acid (aspirin) was used as a model active component drug. When granulated, it was found that increasing of both the liquid to solid ratio (0.8, 1.0 and 1.2) and mixing time (2.5, 5 and 7 minutes) decreased the porosity of the granules. For the dissolution studies, a UV spectrophotometer at 270 nm was used to monitor drug release as a function of time. For the higher porosity granules, i.e. those produced at low granulation time and liquid to solid ratio, dissolution was found to be significantly more rapid. This demonstrates the importance of the granulation process and the resulting granule structure.

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**An investigation on the accuracy and simulation performance of permeability estimation from 3D pore-scale imaging based on the solution of the Laplace's equation****Authors:** Ahmed Zoair<sup>1</sup> ; Jafar Qajar<sup>2</sup> ; Hamed Aghaei<sup>3</sup><sup>1</sup> *aDepartment of Petroleum Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz, Iran*<sup>2</sup> *Digital Rock Physics Research Group, IOR-EOR Research Institute, Shiraz University, Shiraz, Iran*<sup>3</sup> *Affiliated research staff, School of Earth, Atmosphere and Environment, Monash University, Clayton, Australia***Corresponding Authors:** jqajar@shirazu.ac.ir, ahmed.zoair@yahoo.com, aghaei.hamed@gmail.com**Abstract**

Permeability and its distribution play a major role in productive capacity of petroleum reservoirs and hence its prediction is crucial in predicting reservoir performance and determining well production rates. In recent years, the technology of digital rock physics has been introduced as a powerful tool to compute the petrophysical properties of porous materials based on 3D tomographic imaging [1-3]. A variety of methods have been proposed for pore-scale simulation of permeability, of which the most important are the lattice-Boltzmann method (LBM) [4], the classical computational fluid dynamics approaches [5, 6], and the Navier-Stokes solver based on the fast Fourier transform [7]. However, a few studies have focused on development of methods to estimate permeability in reduced computational cost particularly in comparison with the LBM [8-10]. In this study, we present a simple and fast method to calculate permeability of porous materials using 3D pore-scale images based on the solution of Laplace's equation for pressure. An in-house computer program is developed based on finite volume method to determine the distribution of pressure and velocity in voxelated pore space. We use the Euclidean distance map of the pore phase to assign local permeability and a simple upscaling scheme was employed to estimate the permeability tensor. The method was first applied to a range of simple digitized porous media including idealized channels of elementary cross sections, Boolean models of spherical grains, and bundles of capillary tubes and the estimated permeability was then compared to the analytical solutions of idealized microstructure. Next, a new developed solver was used to estimate permeability of digital rocks obtained from  $\mu$ -CT imaging. At the end, the estimated permeability and digitally-computed permeability values were compared using both the Stokes solver and the lattice-Boltzmann methods. Finally, the proposed permeability solver was revealed to be suitable for quick estimation of permeability and rough evaluation of heterogeneity/anisotropy based on  $\mu$ -CT images of rock samples, particularly for large datasets with high number of pore voxels.

**Keywords:** Digital rock physics; Pore-scale imaging; Permeability; Laplace equation; Finite volume; Euclidean distance

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

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## An iterative scheme for two-scale phase-field models in porous media.

**Authors:** Iuliu Sorin Pop<sup>1</sup> ; Carina Bringedal<sup>None</sup> ; Manuela Bastidas<sup>1</sup>

<sup>1</sup> *Hasselt University*

**Corresponding Authors:** [sorin.pop@uhasselt.be](mailto:sorin.pop@uhasselt.be), [manuela.bastidas@uhasselt.be](mailto:manuela.bastidas@uhasselt.be), [carina.bringedal@iws.uni-stuttgart.de](mailto:carina.bringedal@iws.uni-stuttgart.de)

A porous medium is a highly complex domain, in which various processes can take place at different scales. Here we consider a phase-field approach to model the evolution of the evolving interfaces at the micro-scale. After applying a formal homogenization procedure, a two-scale phase-field model is derived, describing the averaged behavior of the system at the Darcy scale (the macro-scale). In this two-scale model, the micro and the macro scale are coupled through the calculation of the effective parameters.

Although the resulting two-scale model is less complex than the original, the usual numerical strategies remain computationally expensive. Here, we propose an adaptive two-scale scheme involving different techniques to reduce the computational effort without affecting the accuracy of the simulations. These strategies include iterations between scales, an adaptive selection of the elements wherein effective parameters are computed, adaptive mesh refinement, and efficient non-linear solvers.

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## An open-source integrated solution for flow and transport in random heterogeneous porous media

**Authors:** Eugenio Pescimoro<sup>None</sup> ; Matteo Icardi<sup>1</sup> ; Federico Municchi<sup>None</sup> ; Marco Bianchi<sup>2</sup>

<sup>1</sup> *University of Nottingham*

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Due to the increasing challenges to preserve water quality and supply at global scale, groundwater flow modeling has become a tool of pivotal relevance for remediation, implementation of policies, and design of applications for recharge management. The strain towards faster and more reliable hydrogeological simulations triggered the development of upscaled and multi-scale approaches employing different diffusion and dispersion models that are still the object of much debate in the community. Our ongoing study focuses on the up scaling of solute transport through heterogeneous geological domains by means of an extensive three-dimensional simulation study, based on a new open-source C++ library, built on top of the well-know finite-volume library OpenFOAM®. We integrate the whole workflow, from geostatistical random field generators to flow and transport solvers with integrated post-processing capabilities. The robustness, scalability and flexibility of the library makes it suitable framework for the development, testing, and application of upscaling techniques. Being the subsurface inaccessible by nature, the appeal to geostatistical techniques is a well-established approach to construct a realistic domain for flow and transport simulations. However, additional challenges are posed by the numerical simulation of highly heterogeneous materials. Indeed, the problem is twofold: on one side it is not always possible to characterize the heterogeneity in a deterministic way, while on the other side numerical methods which are effective for elliptic and parabolic equations solved over homogeneous domains might suffer in heterogeneous media. Both challenges were effectively tackled using the open-source library OpenFOAM whose implementation and capabilities will be illustrated. Preliminary results on flow and transport simulations performed on truncated pluri-Gaussian permeability fields will be shown and the influence of geostatistical metrics (e.g. correlation lengths, variance, geological entropy) on the flow and transport results (e.g. average velocity and breakthrough curves) analysed. Extensions to variable-density, mobile-immobile, and multi-rate mass transfer formulations are also presented in the context of the EU project “SECURE”.

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## **Analysis of droplet mobilization confined in a micro pore-doublet system at low capillary number**

**Authors:** Qumars Azizi<sup>1</sup> ; Amir Alamooti<sup>2</sup> ; Hossein Davarzani<sup>3</sup>

<sup>1</sup> *BRGM (French Geological Survey)*

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Immiscible two-phase flow in porous media has drawn great attention in various applications including soil remediation, enhanced oil recovery, and CO<sub>2</sub> sequestration ( Zarikos et al., 2018; Alamooti et al., 2020). One of the main effective processes on the performance of these applications is the trapped phase mobilization phenomenon. The balance of total drag forces (including pressure and viscose forces) and surface tension forces can determine the mobility of confined droplets (Yang et al., 2019). Several experimental and numerical works have been conducted to quantify and qualify

the mobilization (Madani et al., 2014; Yang et al., 2019). However, the combination impacts of surface hydrophobicity, viscosity ratio, and recirculation on the mobilization of the trapped phase inside the confined droplet at low capillary numbers have less focused.

Here, we use filtered surface force formulation of the volume of fluid method (Raeini et al., 2012) to formulate two-phase flow at microscale at low capillary number. To assess the mobilization process, a 2D pore-doublet model is set and a liquid droplet was confined in one of two micro-channels. This special pore assembly provides an opportunity not only to fully confine a droplet inside one of two microchannels but also to evaluate the role of fluid flow in another microchannel on the mobilization of the confined droplet. We optimized the mesh size using a mesh sensitivity analysis. Then the model was validated against existing experimental data for a droplet partially confined in a microchannel. Furthermore, an analysis was conducted to ensure that the spurious currents are suppressed during the simulation.

We found that regardless of the wettability of the surface, the consideration of the individual critical value for capillary number or viscosity ratio for separation of mobilized and trapped regimes is not efficient. Therefore, a critical line should be considered for both parameters.

However, due to higher surface tension forces for hydrophilic surfaces, this critical line moves to higher values of capillary numbers and viscosity ratios. We performed a force balance analysis on the interface of confined droplet and flowing phase and also on the interface of confined droplet and solid surface for both mobilized and trapped cases. The results show that, regardless of the surface wettability the trapped cases, the total drag forces is equal to surface tension forces. It does not necessarily mean that viscose and pressure forces are in the same direction as the flow of invading phase in the adjacent microchannel can cause negative viscose force against the movement of the droplet. Depending on the viscosity of the confined droplet and the transversal element of viscose force, the recirculation phenomenon can be seen inside the confined droplet.

The results of this work can be used in many applications where the adhesion forces on the walls of pore spaces can play a pivotal role. As a basis, we expect that this model can be coupled with other processes such as heat and mass transfer in more complex porous media where the heterogeneity can influence the mobilization of trapped droplets.

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## **Analysis of the thermal conductance of polymeric ion-exchange membranes**

**Authors:** Sagrario MuñozSan Martín<sup>1</sup> ; V. María Barragán García<sup>1</sup>

<sup>1</sup> *Department of Structure of Matter, Thermal Physics and Electronic*

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The interest on thermal conductance of polymeric ion-exchange membranes is increasingly important due to the growth of new energetic technologies based on transport processes through membranes. The relative importance of the thermal conductance is directly related to the desirability of isolating or enhancing the energy transfer to achieve the optimum performance of diverse membrane-based applications such as fuel cells or electrolyzers. Due to the components in these devices show different thermophysical properties and the junctions between them may be not perfectly flat, most of heat flow passes only through a limited number of pores. So, the actual area of contact is only a small fraction of the nominal or apparent area, and therefore a contact resistance must be taken into account. This thermal contact resistance is related to the thermal conductance.

The aim of this study is to calculate the thermal conductance of commercial polymeric ion-exchange membranes. Different membranes were considered to study the influence of some essential properties such as: the surface heterogeneity, external or internal reinforcement, density, thickness, the ion-exchange capacity or impurity contents, have on the thermal conductance values. For this purpose, a numerical simulation using Comsol Multiphysics® (Comsol Inc., Burlington, MA, USA) that implements the FE numerical technique, was performed using a simple experimental setup previously calibrated. The membrane is sandwiched between two copper cylinders and two probes measure the temperature at both sides of the membrane. The average heat flux along the membranes is also calculated. Thus, the thermal conductance is calculated from the ratio of the temperature drop at the interface to the average heat flux across the membrane.

The results confirm the surface heterogeneity, the reinforcement or the ion-exchange capacity as relevant factors on the thermal conductance value.

Financial support from Banco de Santander and Universidad Complutense de Madrid is gratefully acknowledged.

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## **Analytical Model for Predicting Dynamic Capillary Pressure-Saturation Relationship in Porous Media**

**Authors:** Jawairia Abdul Salik<sup>1</sup> ; Thomas Daniel Seers<sup>1</sup> ; Jassem Abbasi<sup>2</sup> ; Harris Rabbani<sup>1</sup>

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The capillary pressure defined as the pressure difference between the non-wetting and wetting fluid is one of the important parameters that govern the multiphase flow through porous media. Traditionally, the capillary pressure-saturation relationship is determined under equilibrium conditions. However, it has been demonstrated in previous studies, that the dynamic conditions of the system (i.e the rate of flow) can significantly influence the capillary pressure-saturation behavior, and therefore the classical static assumption may not be valid under transient conditions. In this research, we developed an analytical model to study the dynamic nature of the capillary pressure-saturation profile. We extend the Analytical Pore Network Approach (APNA) introduced by Rabbani et al. (2019) to derive a mathematical model for the direct computation of dynamic capillary pressure-saturation relationship in porous media. According to our knowledge, this is a first attempt to analytically predict the dynamic capillary pressure-saturation profile; providing an opportunity for a rapid prediction multiphase flow properties under non-equilibrium conditions. The analytical model was benchmarked against experimental results reported in the literature under various boundary conditions, showing a satisfactory match between the experimental and analytical results.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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## **Analytical Modeling of Mass Transfer Integrating Diffusion and Dispersion in Solvent Injection Based Heavy Oil Recovery Methods**

**Author:** Wanju Yuan<sup>1</sup>

**Co-authors:** Gang Zhao<sup>2</sup>; Chang Su<sup>3</sup>

<sup>1</sup> *Geological Survey of Canada*

<sup>2</sup> *University of Regina*

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An innovative analytical 2D model for solvent injection-based heavy oil recovery was generated with respect to complicated mass transfer mechanisms integrating diffusion and dispersion, dynamic viscosity reduction, and fluids mixture expansion. The high nonlinear process caused by coupled diffusion and fluids movement, viscosity reduction, and mixture volume expansion were analytically captured and analyzed in this model and applied in variable well configurations including single vertical wells and fractured wells.

This proposed analytical methodology is developed by use of the pseudo-pressure and pseudo-time based diffusivity equation linearization, and integral image method (IIM) for whole reservoir scale modeling. The pseudo-time can be converted to the real-time domain by evaluating reservoir average pressure in the region of investigation using IIM. Dynamic mixture volume expansion using linear expansion model was analytically treated as a kind of variable-rate additional source/sink integral within each discretized reservoir domain. Dynamic mass transfer domain and fluids flow pressure domain was coupled analytically in this work and the systematically iterative method was used to make calculation in these two domains as a closed-loop in Laplace domain. Dimensionless terms were used for providing universal solutions. Normalized transient pressure behaviors were calculated and discussed their features in log-log plots.

This method was validated against finely gridded commercial numerical simulation models under limiting cases. The results were well matched and clearly showed fluids mixture expansion acting as an additional source to increase the pressure in porous media compared with the conventional dispersion process. Accordingly, dimensionless pressure and pressure derivative type curves were developed to match flow behaviors, such as radial flow, linear flow, and boundary dominate flow. By comparing with the standard type curve, the mechanism of viscosity reduction and mixture expansion can be quantifiably captured to analyze the expansion features of the solvent and heavy oil mixture, which will become useful tools for accurately evaluating the solvent functional ability in heavy oil recovery methods. A typical cold-oil-production-with-sand (CHOPS) well the configuration of a single fracture structure had been modeled using solvent injection process. Transient pressure behavior with respect to different time domains had been plotted and discussed based on its physical meaning.

This work proposed a new analytical methodology of modeling mass transfer integrating diffusion and dispersion in solvent injection-based heavy oil recovery methods. Solvent diffusion and dispersion, dynamic mixture viscosity reduction, and mixture volume expansion were analytically captured and integrated into reservoir scale modeling using an additional source/sink integral method. This study will also help improve the Post-CHOPS characteristics, and will directly provide operating companies the technique to analyze and have a better understanding of the transient pressure data of solvent injection process in heavy oil recovery methods.

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## Analytical modelling of foam in porous media

**Authors:** Abdallah El Zamli<sup>1</sup> ; Lei Ding<sup>1</sup> ; Kofi Osei-Bonsu<sup>None</sup> ; Harris Rabbani<sup>1</sup><sup>1</sup> *Texas A&M University at Qatar***Corresponding Authors:** abdallah.el\_zamli@qatar.tamu.edu, kofiobonsu@gmail.com, harris.rabbani@qatar.tamu.edu, lei.ding@qatar.tamu.edu

It is reported that approximately only one-third of the original oil in place can be economically recovered from the reservoir after primary and secondary recovery (Osei-Bonsu et al., 2015, p. 520). Miscible gas flooding and steam gas injection, as effective enhanced oil recovery (EOR) techniques, suffer from poor sweep efficiency due to reservoir heterogeneity, gas fingering and gravity override (Farajzadeh et al., 2012, p. 11). Foam EOR has shown a great potential to improve oil recovery throughout the years. Strong foam may have an apparent viscosity that is much higher than that of the gas and liquid; therefore, increasing the gas volumetric sweep efficiency and reducing oil trapping (Shojaei et al., 2018b, p. 1073). Foam flow in porous media is exceedingly complex, which can be defined as a dispersion of gas in liquid separated by lamellae (Osei-Bonsu et al., 2015, p. 520). One of the major complications facing the foam EOR is how to accurately model the foam behaviour in porous media. The two widely used foam models, i.e., the local equilibrium (LE) model and the population balance (PB) model are either physically plausible or computationally expensive. Furthermore, the foam strength is largely dependent on foam texture, which is subsequently determined by water saturation, flow rate, surfactant concentration and pore geometry, etc. However, the influence of pore geometry is not considered in either the LE or PB model. The aim of this research is to propose a novel analytical foam model (AFM) that can predict the apparent viscosity of foam in porous media under complex boundary conditions. By employing the pore geometry data, a better understanding of various properties influencing the foam behavior will be achieved in the AFM model. The AFM model was then validated using existing published experimental data. Overall, we demonstrate a good match between the AFM model and the experimental data, under different foam quality, surfactant concentration and flow rate. The validated AFM model may be further integrated into the reservoir simulation softwares, as it provides a promising tool for reservoir engineers to capture the foam behavior in the reservoir during foam EOR process.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

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## Analytically Derived Upscaled Relative Permeability Curves for Viscous Limit Flow through Layered Porous Media

**Authors:** AbdAllah Youssef<sup>1</sup> ; Stephan Matthai<sup>2</sup>

<sup>1</sup> *The university of Melbourne*

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Layering is widely recognized in geologic porous media at multiple length scales ranging from the micrometer scale to the km scale. Incorporating the impact of the multi-phase flow on such heterogeneity on field-scale simulations demands upscaling not only of absolute permeability, but also the saturation functions; relative permeability and capillary pressure. If done correctly, upscaling of saturation functions preserves the flow features (sweep efficiency and micro-displacement) of the small-scale heterogeneity. Relative permeability upscaling, therefore, is one of the most important steps in reservoir simulation studies.

This study presents a mathematical approach for relative permeability upscaling devised specifically for non-communicating strata. Analytical solutions describe saturation and pressure distribution in each layer in the viscous limit. They are presented in a non-dimensional form derived for both linear and radial flow. Unlike the majority of earlier studies that assume piston-type displacement, our new solutions consider the complexities of frontal advance theory, including the rarefaction waves that follow the sharp flood fronts. However, potential gravity tonguing is ignored. The different multiphase flow properties of each layer (e.g. porosity, permeability, relative permeability endpoints, etc.) are taken into account by our new formulation. Three flow stages, each with its unique time-dependent characteristic variable, are considered for each layer. The overlap among the flow stages in the different layers determines the overall shape of the solution.

Our solutions enable a straightforward evaluation of the dynamics enameled in the relative permeability: the unsteady-state ensembled relative permeability is space-dependent with discontinuities associated with the flood-front saturation jumps. A comparison between the unsteady-state performance and the performance based on the commonly used steady-state upscaled relative permeability curves highlights the inadequacy of steady-state upscaling for viscous-limit flows. It also reveals the capability of the new relative permeability functions to predict the behaviour over the whole flow saturation range, not only for when both phases are mobile between the residual saturations. Beyond the interpretation of laboratory experiments, the applicability of this approach to field-scale simulation is discussed under a newly proposed dual-stage simulation technique.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## **Anomalous nanosilica imbibition in cement-based materials**

**Authors:** Emmanuel Keita<sup>1</sup> ; Badreddine El-Haddaji<sup>1</sup> ; Nicolas Roussel<sup>1</sup>

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Improving the durability and lifespan of concrete transportation infrastructure is a major concern. Penetration of aggressive agents such as chloride ions is known to accelerate structural decay. Several nanotechnology-based treatments intended to decrease permeability are currently under study. The use of nanosilica as a surface treatment has proved to be one possible solution, particularly on aged cementitious infrastructure. The working mechanism is rather unclear as nanosilica may interact in several chemical or physical ways with the concrete composition and microstructure. In this work, we focus on the imbibition of hardened cement paste by colloidal silica suspensions. We monitor the invasion process using an X-Ray scanner. The imbibition of the silica suspension shows anomalous kinetics. Our results suggest that clogging occurs and that the advent of clogging is controlled by a non-trivial relationship between the colloidal particle size and the pore size. A probabilistic clogging model allows us to interpret semi-quantitatively the experimental data. Moreover, nano silica is a source of pozzolan that affects cement hydration and modifies microstructure. As anticipated, the imbibition of water on treated cement paste shows an induction period related to the clogging depth, which significantly slowed the liquid and ionic transfer rate inside the post-treated materials.

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Time Block A (09:00-12:00 CET) **References:**

Roussel N, Nguyen TLH, Coussot P (2007) General probabilistic approach to the filtration process. Phys Rev Lett 98: <https://doi.org/10.1103/PhysRevLett.98.114502> **Acceptance of Terms and Conditions:**

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## Application of Adaptive Conservative Time Integration for Transport in Fractured Porous Media

**Author:** Michael Liem<sup>1</sup>

**Co-authors:** Stephan K. Matthai<sup>2</sup> ; Patrick Jenny<sup>1</sup>

<sup>1</sup> *Institute of Fluid Dynamics, ETH Zurich*

<sup>2</sup> *The University of Melbourne*

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In finite volume methods (FVM) with explicit time integration, the Courant-Friedrichs-Levy (CFL) number needs to be below a critical value in order to ensure stability and accurate time integration. The CFL criterion provides an upper bound of the time step for every grid cell. In conventional methods, where the same time step is used for all grid cells, the lowest value of this upper bound is chosen as the global time step and it can vary over several orders of magnitude throughout the domain. This can lead to an unnecessarily large number of time steps and, in some cases, a prohibitive amount of computational cost.

Various local time stepping schemes have been developed to overcome this drawback. They reduce the number of time integration steps and computational cost by using customized step size for each cell. However, most of them are asynchronous, requiring very small local CFL numbers or the schemes are not strictly conservative. Jenny (2020) introduced a new adaptive time integration scheme for FVM which is conservative, of high spatial and temporal order, robust and easy to implement. The basis for this scheme is that all local time steps  $\Delta t_I$  are fractions of the global time step by powers of two, i.e.,  $\Delta t_I = \Delta t_{Global} / 2^{L_I}$ , where  $L_I \geq 0$  denotes the level of the local grid cell. The grid cells are synchronized after each global time step and strict conservation at the global time resolution is guaranteed. This adaptive conservative time integration (ACTI) scheme is combined with a MUSCL scheme with slope advection to achieve second order accuracy in space and time.

In this work, we apply ACTI to transport through fractured porous media. Typically, the fluid velocity within highly permeable fractures is several orders of magnitudes higher than in the rock matrix. Additionally, local grid refinement might be desirable around fractures. Therefore, the CFL criterion requires very small time steps in the vicinity of the fractures. We show, that ACTI can dramatically reduce the computational cost in such a system compared to conventional (global) time stepping, while the time integration error is much smaller than for implicit schemes.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

JENNY, P. 2020. Time adaptive conservative finite volume method. *Journal of Computational Physics*, 403, pp. 109067. doi: 10.1016/j.jcp.2019.109067 **Acceptance of Terms and Conditions:**

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Poster + / 756

## Application of Convolutional Neural Networks in Flow Simulation of Porous Media: Unsupervised Image Segmentation and Lat-Net for LBM Simulation

**Author:** Hongsheng Wang<sup>1</sup>

**Co-authors:** Dustin Crandall<sup>2</sup> ; Laura Dalton<sup>3</sup> ; Cheng Chen<sup>1</sup>

<sup>1</sup> *Virginia Tech.*

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Three-dimensional high-resolution images, obtained from X-ray micro-computed tomography ( $\mu$ CT) in a non-destructive and non-invasive manner, can be used in digital rock physics (DRP) studies, including property characterization, hydraulic and mechanical behaviour modelling, flow and transport simulation, etc [1, 2]. In recent years, machine learning received great success in various fields of DRP. This work applied two convolutional neural networks to the Lattice-Boltzmann flow simulation: unsupervised image segmentation and Lat-Net for LBM simulation. These two networks can improve the accuracy and efficiency of image segmentation and accelerate the single flow simulation without sacrificing little accuracy. The data is the X-ray  $\mu$ CT image of a sandstone sample, which is first saturated with water, then replaced by supercritical CO<sub>2</sub>.

As a crucial step of standard DRP workflow, image segmentation has a profound impact on the accuracy of follow-up analysis and modelling processes. Recently, supervised learning algorithms for image segmentation have been developed greatly. However, the keystone of those methods is the high-quality label images, which are not always accessible or computationally expensive, and time-consuming to obtain [3]. Nowadays, unsupervised learning algorithms for image segmentation are still under exploration and the design of model architecture is very challenging. W. Kim and A. Kanazaki proposed a brand new convolutional network, following the criteria of image segmentation: '(a) pixels of similar features are desired to be assigned the same label, (b) spatially continuous pixels are desired to be assigned the same label, and (c) the number of unique labels is desired to be large.' [4] This model can optimize the pixel labels based on the representations and the parameters are updated via gradient descent. With the advantage of the convolutional operator to analyze the shape and the pattern of the target, this method showed high accuracy to segment the raw images into three phases: pore space (including water and supercritical CO<sub>2</sub>) and rock grain, in a very short processing time (several minutes per image).

After the image processing and segmentation, apply the Lat-Net [5] to complement the Lattice-Boltzmann method simulation. LBM can be constructed to operate based on the minimum assumptions and modelling the complex materials without geometric simplification [6]. Correspondingly, LBM simulations are extremely computationally and memory demanding. The Lat-Net uses the similarity between LBM simulation and convolutional neural network: for the D2Q9 case, consider the streaming operator as a 3 by 3 convolution and collision step as 1 by 1 convolution. Then, Lat-Net can compress the state size of a simulation and learn the dynamics of this compressed form by using convolutional autoencoders and residual connections in a fully differentiable scheme. After some time step, the steady-state velocity map and permeability resulting from Lat-Net would be compared with the LBPM software package (J. E. McClure) [6], which is a well-developed LBM software.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS19 / 255

## Application of Helmholtz EDL Theory in a Pore Network Model for Studying Capacitive Deionization

**Author:** Michael McKague<sup>1</sup>

**Co-authors:** Hamed Fathiannasab<sup>1</sup>; Mehrez Agnaou<sup>1</sup>; Amin Sadeghi<sup>1</sup>; Jeffrey Gostick<sup>1</sup>

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Research interest in Capacitive Deionization (CDI) as a novel approach for water desalination has increased significantly over the past decade or more. CDI shows significant promise for desalinating brackish or low salinity waters due to a decrease in the energy consumption per ion removed compared to conventional desalination methods such as reverse osmosis [1], [2]. Capacitive Deionization works by storing ions in Electrical Double Layers (EDL) on a pair of oppositely charged porous electrodes. One of the objectives of research surrounding CDI is to increase the salt adsorption capacity of the electrodes used. Past research has shown that pore microstructure has a significant effect on CDI performance including salt adsorption capacity [3]. Pore network modelling is a tool used by researchers in other research areas to study the effect of pore structure on transport in porous media. Pore network modelling uses a resistor in series like network of pores and throats to determine transport properties. Pore network modelling has yet to be utilized in capacitive deionization modelling work. Available capacitive deionization modelling work couples transport equations with appropriate EDL model. The uptake rate of ions into the electrical double layer is determined from EDL theory [4]. It is to the best of our knowledge that no one else has applied EDL theory to a pore network model. Therefore, before a pore network model of a full CDI cell can be developed, appropriate EDL theory must be applied to a pore network model. One such EDL model is the famous Helmholtz model. This was, to the best of our knowledge, the first EDL model to be used in CDI modelling work [5]. Helmholtz assumed a capacitor like EDL structure where charges near the electrode-electrolyte interface are separated and equally compensated. In this work, the application of Helmholtz EDL theory to a pore network model is demonstrated. Electroneutrality in the macropores, equal cation and anion diffusivities, and no flow was assumed simplifying our capacitive deionization model to a transient fickian diffusion algorithm with Helmholtz reaction term coupled with a transient ionic transport algorithm [6]. A pore network simulation was conducted on a small two-dimensional network of 36 pores subdivided into anode, cathode, and spacer pores. OpenPNM was used to do the pore network simulation while COMSOL Multiphysics was used as reference solution to validate the implementation of Helmholtz. The conclusions of this work was that the pore network model correctly applied Helmholtz EDL theory. This is the start of using pore network modelling to study capacitive deionization.

### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS12 / 645

## Application of Lightning Breakdown Simulation in Inversion of Induced Fracture Network Morphology in Stimulated Reservoirs

**Authors:** Hui Zhao<sup>None</sup> ; Guanglong Sheng<sup>None</sup>

**Corresponding Authors:** zhaohui@yangtzeu.edu.cn, shenggl2019@yangtzeu.edu.cn

Accurately characterizing fracture network morphology is necessary for flow simulation and fracturing evaluation. The complex natural fractures and reservoir heterogeneity in shale gas reservoirs make the induced fracture network resulting from hydraulic fracturing more difficult to describe. Existing fracture propagation simulation and fracture network inversion techniques cannot accurately match actual fracture network morphology. Considering the process of lightning breakdown similar as fracture propagation, a new efficient approach for inversion of fracture network morphology is proposed. Based on the dielectric breakdown model (DBM) for lightning breakdown channel simulation and similarity principle, an induced fracture growth algorithm integrating reservoir in-situ stress, rock mechanical parameters, and stress shadow effect is proposed. The fractal index and random function are coupled to quantitatively characterize the probability distribution of induced fracture growth path. At the same time, a matching rate function is proposed to quantitatively evaluate the fitting between fracture network morphology and the micro seismic data. Combined with automatic history matching method, the actual fracture network morphology can be inverted with the matching rate as objective function. The proposed approach is applied to fracture network simulation of fractured horizontal wells of shale oil reservoir in the Lucaogou Formation in Xinjiang of China, and the fracture networks from inversion fit well with the micro seismic data. A simulation of 94 fractures in the 32 section of Well X2 in Xinjiang Oilfield shows that the well develops more obvious branch fractures. The single-wing fracture network communicates approximately 200m horizontally and approximately 10m vertically. When simulating a single fracture in a production well, it is necessary to consider the influence of complex fracture network morphology, but when simulating a single well or even a reservoir, only the main fracture needs to be considered. This paper proposes an induced fracture growth algorithm that integrates reservoir in-situ stress, rock mechanical parameters, and stress shadowing effects. This algorithm greatly improves the calculation efficiency on the premise of ensuring the accuracy of induced fracture network morphology. The approach in this paper provides a theoretical basis for flow simulation of fracturing reservoirs and optimization of fracture networks.

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## Application of the Virtual Element Method to Two-phase Flow of Immiscible Fluids in Porous Media

**Authors:** Martina Busetto<sup>1</sup> ; Stefano Berrone<sup>2</sup>

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The Virtual Element Method (VEM), firstly introduced in [1], is a very recent extension of the Finite Element Method that allows the resolution of partial differential equations using general polygonal grids. This brings forth several advantages including better domain meshing and approximation of geometric features that are of great relevance in tackling problems characterized by complex geometries. Despite the growing interest in testing the performance of this new numerical method on physical and engineering problems characterized by challenging domains, still very few applications exist to complex and realistic geological flow models in porous media. In this framework, the aim of the present contribution [2] is to investigate the potentialities of the VEM in the contest of two-phase flow of immiscible fluids in porous media, a problem described by a system of time-dependent coupled nonlinear partial differential equations. In this work we discretize the equations in time and in space using an iterative IMPLICIT-Pressure-IMPLICIT-Saturation method coupled with a primal  $C^0$ -conforming VEM. We investigate the performance of the resulting fully discrete scheme showing its potentialities in terms of simplified construction of high-order approximations and mesh flexibility, a very attractive feature for the numerical modeling of two-phase flow processes in fractured porous media. The method is tested both on a problem with known analytical solution and on some more realistic benchmark problems that are of interest for engineering applications in porous media [3].

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS25 / 293

## Applications of Physics Informed Neural Networks for Modeling Soil Water Dynamics

**Authors:** Toshiyuki Bandai<sup>1</sup> ; Teamrat Ghezzehei<sup>1</sup>

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The Richardson-Richards equation (RRE), a nonlinear partial differential equation (PDE), is commonly used to describe soil water dynamics. Analytical solutions of RRE are available only when simplifying assumptions are made. Therefore, numerical methods, such as the finite difference, finite element, and finite volume methods, are employed when solving practical problems. Here, we introduce an alternative numerical method known as physics-informed neural networks (PINNs), in which neural networks approximate the solution to the RRE. The PINN approach, which is rapidly gaining popularity in various fields of physics, is based on the universal approximation theorem that neural networks with at least one hidden layer with a finite number of weights can approximate any continuous function arbitrarily well. Furthermore, the automatic differentiation allows the evaluation of the residual of PDEs, which is incorporated into the loss function to be minimized. Although the forward solution of PDEs using PINNs is computationally more expensive than other numerical methods, the PINNs approach is expected to be more effective for the inverse problem because it does not require a repetitive solution of the forward problem as in other numerical methods. We

will present a PINNs solver for the RRE and compare its approximations with analytical and conventional numerical solutions for homogeneous and layered soils. We also present a PINNs method for approximation of soil surface flux from only near-surface soil moisture measurements, which demonstrates the superior potential of PINNs for solving inverse problems.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

Bandai, T. and T. A. Ghezzehei. "Physics-informed neural networks with monotonicity constraints for Richardson-Richards equation: Estimation of constitutive relationships and soil water flux density from volumetric water content measurements." *Water Resources Research*, 57(2): e2020WR027642, 2020. <https://doi.org/10.1029/2020WR027642> **Acceptance of Terms and Conditions:**

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MS15 / 90

## Applying Machine Learning Methods to Speed Up Two-Phase Relative Permeability Upscaling

**Authors:** Yanji Wang<sup>1</sup> ; Hangyu Li<sup>1</sup> ; Jianchun Xu<sup>1</sup> ; Ling Fan<sup>1</sup> ; Xiaopu Wang<sup>1</sup> ; Shuyang Liu<sup>1</sup>

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Traditional flow-based two-phase upscaling entails the computation of upscaled relative permeability functions for each coarse block or interface. It can be very time-consuming especially for large models with a large quantity of coarse grid blocks or for cases that requires simulation runs over multiple geological realizations (as commonly used in uncertainty quantification or optimization). In this work, we introduce machine learning (ML) methods into the two-phase upscaling procedure to significantly speed up the upscaling computations. In the new procedure, the flow-based relative permeability upscaling is performed only for representative coarse blocks/interfaces, while the upscaled functions for the majority of the coarse blocks are provided by the ML methods.

The new upscaling procedure entails a few steps. First, a ML method is applied to select the representative coarse blocks/interfaces based on the static permeability distribution associated with the target regions. Flow-based two-phase upscaling is then performed for the selected blocks/interfaces to build a database. A different ML model can then be constructed to reveal the relationship between the upscaled relative-permeability functions and the corresponding static permeability distribution. This ML model is finally used to give the upscaled relative permeability functions for the rest of the coarse blocks/interfaces. In this work, both the local and extended local two-phase upscaling approaches with generic pressure and saturation boundary conditions and effective flux boundary conditions are incorporated with the ML-based upscaling procedure.

We test the new upscaling procedure for generic (left to right) flow problems using 2D models for oil-water two-phase systems. Both Gaussian and channelized permeability fields are considered. Extensive numerical results have shown that the coarse-scale simulation results using the ML-based upscaling procedure are of similar accuracy compared to those using full flow-based upscaling. The relative errors of the total production rate and water cut are within 5%. Besides, at least one order of magnitude speedups achieved, which are quite significant. Higher speedup is observed for models with larger dimensions.

The ongoing work includes extending the procedure into 3D models, and testing it for actual field problems with more complex model geometry.

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Poster + / 296

## Applying Reaction-Diffusion Models to Analyse Turing Patterns on Batteries

**Authors:** Rebecca Inkpen<sup>None</sup> ; Anotida Madzvamuse<sup>None</sup> ; Benedetto Bozzini<sup>None</sup>**Corresponding Authors:** benedetto.bozzini@polimi.it, a.madzvamuse@sussex.ac.uk, rci20@sussex.ac.uk

This paper investigates the spatial patterns of metal deposit on battery cathode by electrodeposition during use. This is done by modelling with a reaction-diffusion system on a finite two-dimensional domain and examining the conditions required for Turing instability. Turing instability requires analysing the stability of the system allowing for diffusion and also without diffusion. Phase portraits are produced as well as basins of attractions for parameter values for the diffusion-less system. The full system is discretised using the Finite Element Method and then solved numerically. Tests are carried out to see the effects of different variable values on the resulting spatial patterns.

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MS18 / 506

## Assessment of the role of densification on the displacement of DNAPL in high permeable porous media using a polymer solution

**Authors:** Amir Alamooti<sup>1</sup> ; Stéfán Colombano<sup>2</sup> ; Sagyn Omirbekov<sup>3</sup> ; Azita Ahmadi-Sénichault<sup>4</sup> ; Hossein Davarzani<sup>5</sup><sup>1</sup> *Institut de Mécanique et Ingénierie de Bordeaux (I2M), Arts et Métiers Institute of Technology, CNRS, and BRGM(French geological survey)*<sup>2</sup> *BRGM (French Geological Survey)*<sup>3</sup> *Institut de Mécanique et Ingénierie de Bordeaux (I2M), Arts et Métiers Institute of Technology, CNRS, and BRGM(French Geological Survey)*<sup>4</sup> *Institut de Mécanique et Ingénierie de Bordeaux (I2M), Arts et Métiers Institute of Technology, CNRS*<sup>5</sup> *BRGM(French Geological Survey)***Corresponding Authors:** a.alamooti@brgm.fr, h.davarzani@brgm.fr, azita.ahmadi@ensam.eu, s.colombano@brgm.fr, s.omirbekov@brgm.fr

The remediation of sites contaminated with Dense Non-Aqueous Phase Liquids (DNAPL) has gained great prominence due to the extreme difficulty of their remediation (Colombano et al., 2021). These

DNAPLs, subjected to gravity forces, penetrate downwards through the aquifer and form a discontinuous insoluble trapping phase below the groundwater level. On the one hand, owing to their high density, high interfacial tension and high viscosity, the direct pump-and-treat method is not efficient enough to extract DNAPLs from the pore spaces. On the other hand, because of dissolution and stability issues, some other conventional remediation techniques such as surfactant or foam injection are not applicable (Maire et al., 2018; Omirbekov et al., 2020). Although using polymers can improve DNAPLs displacement by increasing the viscose pressure, in the case of high-density DNAPLs the gravity forces can overcome the viscose forces (Miller et al., 2000). Furthermore, because of the high permeability of the porous media, the capillary forces cannot prohibit the upward movement of polymer solution due to density contrast between the polymer and DNAPLs.

Here, we evaluated the rheological behavior of various polymer solutions (guar gum, xanthan gum, and carboxymethyl cellulose (CMC)) to find the most appropriate one to be able to suspend barite( $\text{BaSO}_4$ )-polymer solution. We employed a new formulation of densified CMC polymer solution to displace DNAPLs from the porous media. To examine the role of densification of the polymer solution we used barite in different concentrations equivalent to various ranges of densities (from 0.6 up to 1.15 times the density of DNAPL). In this regard, using a decimetric-scale 2D-sandbox, we designed an experimental procedure with similar permeability and fluids configuration as in the real site. To evaluate the efficiency of the displacement of the DNAPL by the densified polymer solution, the solution was injected through the DNAPL at the bottom middle of 2D-sandbox, for different solution densities but at a fixed injection rate. The injection was monitored using an advanced imaging technique and mass balance interpretation.

The results showed that the denser the polymer solution, the more significant is the lateral movement of DNAPL. In contrast, when polymer solutions with a lower density are used, the gravity forces cause more vertical displacement. The analysis of displacement efficiency depicts that when the density of polymer-barite solution is close to the density of DNAPL, the mobilization of trapped DNAPL is improved up to 150% in comparison to using only polymer or other solution densities. To model the displacement of two-phase flow, generalized Darcy's law and continuity equations were employed. The developed model predicts well the experimental fluid-fluid interface (image analyzing) as well as the displacement efficiency.

Our new formulation of the polymer solution can result in a great improvement in remediation processes of soils contaminated with DNAPL as it is presumably a safe and stable mobilization technique. We anticipate that our model can be considered as a good cornerstone for more complicated cases where the role of non-Newtonian behavior of polymer solution and the polymer retention inside the porous media can be involved.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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**Poster + / 9**

## **Assessment of two hydraulic models of canal of Calais regarding the control issue**

**Authors:** Roza Ranjbar<sup>1</sup> ; Eric Duviella<sup>2</sup> ; Lucien Etienne<sup>2</sup> ; Jose Maria Maestre<sup>3</sup>

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Hydrographical systems which are mainly comprised of dams, rivers, channels, etc. are in the category of large-scale networks. These systems are not only complex systems in case of consisting of different hydraulic devices such as pumps or gates, but also they are in exposure to complicated circumstances like different demands, unknown inputs, drought periods, rainfall, and floods. Thus for answering the users' demands, assuring the demanded water levels and avoiding/limiting the probable flooding, applying a control strategy is of importance. Thanks to the recent advances in automation and computing science, there are several tools and methods to assist humans in case of the control issue. Additionally, another important item to be considered prior to control is the case of modeling and simulations. A hydraulic model can be used to estimate the unknown inputs and by having an accurate hydraulic model, it is possible to precisely determine the discharges and levels. Afterward, the hydraulic model is connected to software such as Matlab and the required codes so that the control strategies could be implemented and tuned. In the domain of water systems, model predictive control (MPC) has been widely used and received much attention and popularity due to the principle behind that, for applying the dynamic model of the system for predicting the impacts of the unknown inputs. MPC is also practical in the mentioned domain because of its ability to operate properly in the existence of constraints. MPC is compatible with various hydraulic models of the open-flow channels which basically work with Saint Venant equations and in this regard, considering the delay and attenuation in the wave propagation are crucial. In the matter of hydraulic modeling, there are some solutions such as SIC<sup>2</sup>, Hydra, Mike11, SWMM, HEC-RAS, etc. Among these solutions which most of them can link to GIS (Geographic Information System), few of them are linked to Automatic software like Matlab. Based on simulation architectures, the objective of the presented paper is to define the main differences in the application of two software of SIC<sup>2</sup> and HEC-RAS in the real-data based simulation of the canal of Calais regarding using MPC for controlling over the canal.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Segovia, P., et al. "Model predictive control and moving horizon estimation for water level regulation in inland waterways." *Journal of Process Control* 76 (2019): 1-14.

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Ranjbar, R, et al. "Framework for a digital twin of the Canal of Calais." *Young Scientists Conference in Computational Science* (2020). **Acceptance of Terms and Conditions:**

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**MS10 / 518**

## **Automatic cracks detection in 3D $\mu$ CT images using DVC total variation strain regularization**

**Author:** Zaira Manigrasso<sup>1</sup>

**Co-authors:** Jan Aelterman<sup>1</sup> ; Wilfried Philips<sup>1</sup>

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This work aims to automatically detect the location of cracks formation during uniaxial compaction experiment of grain assemblies using a robust and novel Digital Volume Correlation (DVC) approach.

Experiments, such as absorption or compression, can lead to abrupt structural modifications of the material (e.g., swelling, tears or cracks), that demand robust algorithms to be detected and quantified. Over the years, many techniques have been developed for cracks detection and measurements. Some of them are based on variation of gray scale or color pixel intensities (direct measurements) [1], others are based on the results of Digital Volume Correlation (DIC) (indirect measurements) [2][3], most of these techniques are developed for 2D dataset. In many cases visual inspection is still in use [4].

DVC, based on the theory of DIC [5], but developed for 3D dataset, is a technique for displacement field measurements from which strain field is calculated. DVC is an ill-posed problem: multiple displacements can lead to a data-accurate and a good quality registration of images. Therefore, to distinguish realistic from unrealistic displacement, prior knowledge may be introduced in the form of a regularization term. In the case of grains aggregates the structure of the sample is heterogeneous and, therefore, it is plausible that during compression experiments each component of the sample has its own response in terms of strain (heterogeneous strain). Given the hypothesis of strain heterogeneity, the regularization term may be thought as a term that defines a piecewise constant strain penalizing the total variation (TV) of the strain. TV strain regularization method copes also with the presence of noise in the local strain field. Local strain is indeed computed based on the local variation of the displacement field (i.e., gradient of the displacement), therefore it is very sensitive to small noisy variations in the displacement field. Often the solution to this problem is the application of a smoothing filter [6] [7]. Filtering, in some cases, may be counterproductive: if on one hand it reduces the noise, on the other hand it reduces the resolution of the strain field and that is not a desired effect for cracks detection in  $\mu$ Ct dataset [3].

Micro-CT dataset used in [8], obtained through the Yoda portal of Utrecht University, has been acquired during a compaction experiment on quartz assemblies at room temperature and dry condition. The compression has been performed at different loads (20 MPa- 25 MPa- 50Mpa).

The method proposed in this paper can identify automatically, with high accuracy and high resolution, the location of the cracks in the grains.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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## Averaged Models for Two-Phase Flow in a Pore: The Effect of Hysteretic and Dynamic Contact Angles

**Authors:** Stephan B. Lunowa<sup>1</sup> ; Carina Bringedal<sup>None</sup> ; Iuliu Sorin Pop<sup>2</sup>

<sup>1</sup> Hasselt University, Computational Mathematics (CMAT)

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We consider a model for the flow of two immiscible fluids in a two-dimensional thin strip and in a three-dimensional tube of varying width. This represents an idealization of a pore in a porous medium. The interface separating the fluids forms a freely moving interface in contact with the wall and is driven by the fluid flow and surface tension. The contact line model incorporates Navier-slip boundary conditions and a dynamic and possibly hysteretic contact angle law.

We assume a scale separation between the typical width and the length of the thin strip. Based on asymptotic expansions, we derive effective models for the two-phase flow. These models form a system of differential algebraic equations for the interface position and the total flux. The result is Darcy-type equations for the flow, combined with a capillary pressure - saturation relationship involving dynamic effects.

Finally, we provide some numerical examples to show the effect of a varying wall width, of the viscosity ratio, of the slip boundary condition as well as of having a dynamic contact angle law. Furthermore, we compare the effective model to experimental data for the capillary rise in tubes.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

S. B. Lunowa, C. Bringedal, and I. S. Pop, On an averaged model for immiscible two-phase flow with surface tension and dynamic contact angle in a thin strip, *Studies in Applied Mathematics*, (2021). Accepted. UHasselt preprint available at [uhasselt.be/Documents/CMAT/Preprints/2020/UP2006.pdf](https://uhasselt.be/Documents/CMAT/Preprints/2020/UP2006.pdf). **Acceptance**

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MS7 / 119

## BDDC for MHFEM discretization of unsteady two-phase flow in porous media

**Authors:** Jakub Solovský<sup>1</sup> ; Radek Fučík<sup>2</sup> ; Jakub Šístek<sup>3</sup>

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<sup>2</sup> Czech Technical University in Prague

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This work deals with the application of the Balancing Domain Decomposition based on Constrains (BDDC) method to unsteady two-phase flow problems in porous media.

We briefly describe the spatial discretization of the problem which is based on the mixed-hybrid finite element method (MHFEM) and semi-implicit time discretization.

Then, we describe the BDDC method, in detail discuss the differences between the symmetric and non-symmetric cases, and present necessary modifications of the algorithm for the more complicated non-symmetric case. We describe the parallel implementation of the method and highlight the critical steps of the algorithm that affect the performance and scalability.

The parallel implementation is then tested on benchmark problems in 2D and 3D and its efficiency is investigated on various meshes.



The numerical results indicate that the method preserves high computational efficiency for increasing number of processes and, therefore, allows solving problems on very fine meshes. In the case of unsteady problem, additional speedup is achieved using the information from previous time steps for the solution in the current time step.

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Poster + / 751

## **Bacillus subtilis, A Plant Growth Promoting Rhizobacteria, Improves Soil Hydro-Physical Properties**

**Authors:** Fatema Kaniz<sup>1</sup> ; Yan Jin<sup>1</sup> ; Harsh Bais<sup>1</sup><sup>1</sup> *University of Delaware***Corresponding Authors:** hbais@udel.edu, fkaniz@udel.edu, yjin@udel.edu

*Bacillus subtilis* is a well-known plant-growth-promoting-rhizobacteria (PGPR). It has been suggested that PGPR influences the hydro-physical properties of soil, but the mechanistic understanding of this is still scarce. As a stress-tolerant-bacteria, *Bacillus subtilis* can produce biosurfactant to create surface-tension and viscosity gradient and thus form and spread visco-elastic biofilm in order to cope with the fluctuating water conditions of the soil. This, in turn, can affect the hydraulic and interfacial properties of soil. Understanding the ecological significance of such a strategy and identifying some key missing links of the important physicochemical traits of EPS (Extra-cellular Polymeric Substances) and biofilm to soil physics and hydraulics were the motivation of this work. We conducted evaporation, percolation, and pellicle experiments on the wild-type and its EPS-knock out (eps-) and surfactin-knock out (sfp-) mutants-treated sands to identify key mechanisms responsible for EPS' (and PGPR's) potency on water retention. Our results show that EPS produced by the *Bacillus subtilis* can increase water retention of fine sands by reducing the upward (evaporation loss) and downward (percolation) flow of water. Interrupted capillarity, increased sorption and hydraulic decoupling are likely the causative mechanisms here. SEM-imaging and water repellency data suggest that the occurrence of hydraulic stability rather than mechanical stability in imparting such an outcome. Our study highlights the importance of flow-related variables of surface tension, viscosity, and water repellency to understand the water retention phenomena in a low Reynold's number condition. These research outcomes would contribute to the fundamental understanding of early-stage-biofilm mediated hydro-physical changes of soil and thereby provide a scientific basis for developing biofilm strategies that could effectively manage soil-water in order to achieve sustainability in agriculture.

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MS14 / 584

## Bayesian Inference of Poroelastic Properties from Induced Seismicity Data Using an Energy-based Poromechanics Model

**Author:** Mina Karimi<sup>1</sup>

**Co-authors:** Mehrdad Massoudi<sup>2</sup> ; Matteo Pozzi<sup>3</sup> ; Kaushik Dayal<sup>3</sup>

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Deep water injection related to shale gas extraction is increasingly relevant for the energy sector. Injected fluids in porous deformable elastic media increase pore pressure, reduce normal effective stress, and change the available friction along fractures and faults. Consequently, slip can occur, causing seismic events. Understanding this mechanism and identifying the stress field around the injection wellbores play a central role in assessing the seismic hazard. One of the crucial steps is inferring the unknown model parameters (i.e. poroelastic properties) from the noisy data of injection sites. Due to the indirect relation between the uncertain parameters and the empirical observation (i.e. number of earthquakes and stress drop variations in injection sites) and the high dimension of parameters' domain, the inverse problem is computationally expensive. In this work, we develop a nonlinear forward model by formulating a variational continuum framework of multi-component poromechanics to characterize the evolution of stress, pore pressure, and other mechanical quantities. We adopt a Bayesian inference framework to integrate the partial differential equations (PDEs) of the forward mechanical model with models of uncertainty for observation and parameters. The Bayesian framework provides a probabilistic characterization of the unknown parameters of the physics-based model by updating the prior knowledge of these parameters based on the noisy measurements of injection sites. Maximizing the updated probability distribution or the posterior distribution provides the solution of high-dimension inverse problem. To quantify the uncertainty and predictability of the Bayesian method's solution, we investigate sampling algorithms and their challenges to explore the high-dimension parameter spaces. We use the accelerated Markov Chain Monte Carlo (MCMC) algorithms using the local gradient and Hessian (of the posterior) information to get samples from the posterior distribution.

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MS7 / 629

## Benchmark of different coupling schemes for reactive transport in saturated porous media

**Authors:** Vanessa Montoya<sup>1</sup> ; Renchao Lu<sup>1</sup> ; Jaime Garibay-Rodriguez<sup>1</sup> ; Thomas Nagel<sup>2</sup> ; Dmitri Naumov<sup>3</sup> ; Haibing Shao<sup>4</sup> ; Olaf Kolditz<sup>5</sup>

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The development of continuum reactive transport models in porous media traces back to mid-80's when the theoretical framework to consider reactions in mass transport equations was outlined. Since their establishment, the operator-splitting (OS) approach has been frequently used due to its easy implementation and computational efficiency in large scale simulations including complex chemical processes. Existing and widely used OS-finite element framework in reactive transport normally adopts different collocation schemes for spatially discretizing the transport (i.e. advection and diffusion) and the reaction term of the advection-diffusion-reaction equation. While this numerical approach in general works well in homogeneous systems, it may fail if the field variables (i.e. concentration, hydraulic pressure) vary rapidly, for example, close to the domain boundaries or in the interfaces between different materials. In these cases sharp gradients exist and standard numerical schemes normally lead to inaccurate and unstable numerical results.

A novel OS-finite element framework adopting a consistent collocation scheme of all the field variables in the integration points has been recently developed in our group, validated and implemented in OpenGeoSys-6 (Lu et al. (2021)). Contrary to previous finite element OS-schemes, the reaction term was calculated at the integration point level, instead of the nodes where a chemical solver (i.e. Phreeqc) was called for the chemical speciation calculation. Verification of the new implementation was done by comparing the results with different analytical solutions including a first order bio-degradation reaction and a coupled transport-dissolution processes and feedback on porosity changes. In this study, we extend the validation of the method by benchmarking different numerical coupling schemes and comparing the results to experimental observations obtained in a) a well-controlled laboratory scale column experiment including a dissolution reaction with feedback on porosity changes and b) through diffusion experiments of sorbing cations in clay.

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Lu et al. (2021) Water Resources Research (submitted) **Acceptance of Terms and Conditions:**

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MS10 / 33

## Benchmarking Conventional and Machine Learning Segmentation Techniques for Analysis of Digital Rock Physics Properties

**Author:** Marcel Reinhardt<sup>None</sup>

**Co-authors:** Arne Jacob ; Michael Kersten<sup>1</sup> ; Frieder Enzmann ; Francesco Cappuccio<sup>2</sup> ; Pit Arnold ; Olga Moravcova<sup>3</sup>

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Image segmentation remains the most critical step in Digital Rock Physics (DRP) workflows, affecting modelling results and the analysis of physical rock properties. Conventional segmentation techniques struggle with numerous image artefacts and user bias, which lead to considerable uncertainty. This study evaluates the advantages of the machine learning algorithm of the Ilastik code to DRP problems. Images of porous and fractured samples were acquired by X-ray computer tomography and segmented by both conventional methods (thresholding, watershed), and a machine learning approach. Porosity, permeability, flow fields, and preferred flow paths were computed. For each fracture segmentation, two skeletonized 3D images were calculated providing information about the true aperture distribution and orientation variation. Mean mechanical aperture and roughness were

obtained from these aperture data. Additionally, the uncertainty of the pixel classification segmentation was calculated. A comparison with conventional segmentation methods highlight the superior capabilities of the machine learning approach, which does not even need excessive amounts of training data. Instead, these data can be provided by the user directly on the images, where a constant feedback with the output of Ilastik minimizes user bias. The program is easy to use, resource saving, and provides for high quality segmentations and uncertainty calculations as a quantitative measure for evaluating the output. For our rock samples, the machine learning segmentation was able to handle all artefacts and complexities without prior filtering. A comparison of the described methods highlights the importance of a high-quality segmentation if considerable variations in physical rock properties are to be considered.

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MS13 / 493

## Beyond tortuosity: evaluating connectivity in multimodal catalysis supports

**Authors:** Marc Fleury<sup>1</sup> ; Gerhard Pirngruber<sup>1</sup> ; Aleksandra Glowska<sup>1</sup> ; Leonor Catita<sup>1</sup> ; Thibaud Chevalier<sup>1</sup> ; Elsa Jolimaitre<sup>1</sup>

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The diffusion properties are a key parameter for catalysis supports. These properties are often gathered in one single parameter called tortuosity defined as the ratio of the bulk to the effective diffusivity on a given liquid or gas diffusing inside the porous media. The tortuosity parameter is expected to depend on the geometry of the porous network without chemical interaction of the molecules with the solid surface. However, for complex composite support materials comprising, for example, microporous zeolites and mesoporous oxide binders, the tortuosity concept is not sufficient for describing the transport properties as it might also depend on pore size, type of liquid and surface properties [1–4]. More detailed information about the connectivity between the different pore compartments and the limiting transport steps is needed. In this work we deal with hydrocracking catalysts supports as a study case. These systems contain a wide distribution of pore sizes spanning from microporosity (2 types of zeolites), mesoporosity induced by the alumina binder and macroporosity introduced during the shaping procedure. The question is to determine in which system the meso and macroporosity provide the best access to microporosity.

For this purpose, we used various NMR techniques at low field: NMR cryoporometry to determine pore size distribution in the range 2 nm to 1 micron and the amount of microporosity [5,6], standard PFG-NMR to determine diffusion coefficients, T1 and T2 relaxation time distribution and relaxation exchange spectroscopy (REXSY [7]) to evaluate diffusive exchange between porous compartments. Different fluids were used: water, cyclohexane, squalane and 2-propanol. We varied also the temperature up to 90°C. Diffusive exchange is best revealed in T2-exchange-T2 maps (see figure) when the diffusion length is limited or when the solid-liquid interactions are strong, for example using squalane or 2-propanol respectively. The analysis of these maps allows quantifying the exchange time and compare catalysis supports in terms of diffusive transport, in addition to tortuosity.

The two studied samples labeled A and B vary essentially by the nature of zeolite used. A and B have respectively a specific surface of 843 and 727 m<sup>2</sup>/g. The measured exchange time (with squalane) between micro and mesoporosity was similar for both A and B, but the relative amount of exchanged molecules was larger for B. Hence while B is less porous and slightly more tortuous with a smaller surface, it has better local transport properties than A. The relation between the transport properties of these hierarchical systems and the characteristics of the zeolites constituting A and B will be analyzed in detail.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

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## **Block Copolymer Ultrafiltration Membranes: Stochastic Microstructure Delineation and Flow Simulation**

**Authors:** M. Sadegh Riasi<sup>1</sup> ; Lilly Tsaour<sup>2</sup> ; Ulrich Wiesner<sup>2</sup> ; Lilit Yeghiazarian<sup>1</sup><sup>1</sup> *University of Cincinnati*<sup>2</sup> *Cornell University***Corresponding Authors:** yeghialt@ucmail.uc.edu, lt448@cornell.edu, ubw1@cornell.edu, riasimh@ucmail.uc.edu

Block copolymer ultrafiltration membranes have a wide range of applications from drug delivery to water purification and virus filtration. Although optimizing flow is critical to the performance of such ultrafiltration membranes, little success has been reported on their numerical flow characterization. The main challenges have been reported as i) hierarchical pore structure delineation and ii) lack of an image-based micro-scale modeling approach that is computationally efficient and that can capture such wide pore size distribution. In this study, we address the challenge of pore structure delineation using an array of SEM images with different resolutions. Segmenting the SEM images using continuous max-flow and min-cut algorithm, they are used to collectively determine the pore size distribution and pore density profile of the membrane. To compute permeability, a novel stochastic pore network model (SPNM) is proposed and absolute permeability of two block copolymer membranes is then computed and compared with the experimental measurements.

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## Block-partitioned solvers for poromechanics via gradient flows and minimization

**Authors:** Jakub Both<sup>1</sup> ; Kundan Kumar<sup>1</sup> ; Jan Martin Nordbotten<sup>1</sup> ; Florin Adrian Radu<sup>2</sup>

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Dissipative processes can be often modeled as gradient flows, closely related to thermodynamical principles; flow in deformable porous media e.g. modeled by the Biot equations also falls into this category. A gradient flow structure can have various benefits including access to the well-posedness analysis or development of numerical solvers by employing abstract mathematical tools and concepts.

In this talk, we focus on the development of block-partitioned solvers for coupled poromechanics from a gradient flow perspective [1]. After time discretization, a gradient flow structure translates to an optimization structure. Ultimately, robust solvers can be developed by application of alternating minimization, which are widely applied in convex analysis. Convergence can be studied by employing abstract tools, resulting in sharp convergence rates. This approach covers previous results and methods (e.g. fixed-stress and undrained split) for the well-studied Biot equations, previously obtained by case-specific analyses. Yet, our approach extends to a more general class of poromechanics problems and enables a systematic approach for extensions involving e.g. viscoelastic effects, permeability multiple-network poroelastic effects, and nonlinear effects, among others.

### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

[1] Both, J.W., Kumar, K., Nordbotten, J.M. and Radu, F.A., 2019. The gradient flow structures of thermo-poro-visco-elastic processes in porous media. arXiv:1907.03134. **Acceptance of Terms and Conditions:**

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MS21 / 684

## Bounds for effective Forchheimer coefficient in randomly heterogeneous porous media

**Authors:** Valentina Ciriello<sup>1</sup> ; Alessandro Lenci<sup>2</sup> ; Farhad Zeighami<sup>3</sup> ; Vittorio Di Federico<sup>3</sup>

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An understanding of the interplay between non-linear effects in porous media flow and domain heterogeneity is of great importance in several engineering and geological applications.

For a one-dimensional, statistically heterogeneous medium, we investigate non-linear flow caused by a uniform external pressure gradient, and described at the local scale by the Forchheimer equation; in the latter, the inertial effects are represented by adding to Darcy's law an additional term proportional to the fluid density and to the second power of the flow rate.

Since most experimental values of Forchheimer coefficient have been derived at the laboratory scale, a formula for its upscaling is much needed for the interpretation of field results in heterogeneous aquifers, when there is a reason to include nonlinear effects.

The permeability is considered a spatially homogeneous and correlated Gaussian random field with a given PDF, while the local Forchheimer coefficient  $\beta$  is related to the local permeability  $k$  value via the empirical inverse power-law correlation  $\beta = a/k^c$ , suggested in the literature on the basis of experimental data, with  $a$  a constant and  $c$  an exponent in the range 0-2. Under the ergodic hypothesis, the effective permeability and Forchheimer coefficient are derived for two one-dimensional flow geometries: flow parallel to permeability variation (serial-type layers), and flow transversal to permeability variation (parallel-type layers); the expressions derived for the effective Forchheimer coefficient generalize those derived in the past for a discrete parameter variation. For the effective permeability, the classical results derived in the context of Darcy flow are recovered: the harmonic and the arithmetic mean respectively for the series and parallel arrangement.

For serial-type layers, an expression for the effective Forchheimer coefficient is derived in closed form; for parallel-type layers, an approximate analytical expression is derived under the hypothesis of small values of a dimensionless number  $Z$  including the pressure gradient. For higher values of  $Z$ , the effective Forchheimer coefficient is derived numerically. Upon comparing the results, the validity of the approximate numerical solution is assessed. The impact of the adoption of different shapes of the permeability PDF (lognormal or gamma) is also investigated.

As medium heterogeneity increases, the effective Forchheimer coefficient  $\beta_{eff}$  is found to increase for both geometries examined; for serial-type layers, it is also an increasing function of the exponent  $c$ ; the opposite is true for parallel-type layers. The effective Forchheimer coefficient  $\beta_{eff}$  is also moderately sensitive to the shape of the permeability PDF adopted.

Our results allow to evaluate the error made in the calculation of  $\beta_{eff}$  when the mean permeability value is inserted in the empirical correlation; the relative error increases with medium heterogeneity and can easily be in the range 10-100.

Results obtained for two limit geometries (serial- and parallel-type layers) in 1-D provide lower and upper bounds for the evaluation of the effective Forchheimer coefficient in 2-D flows. Results for 2-D isotropic domains can be derived heuristically via an averaging procedure of the corresponding 1-D expressions such as the geometric mean. Preliminary direct numerical simulations in 2-D agree fairly well with the proposed heuristic formulation.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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Poster + / 243

## Bulk and interfacial properties of alkanes in the presence of carbon dioxide, methane, and their mixture

**Author:** Arun Kumar Narayanan Nair<sup>1</sup>

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Currently, more than 30 Gt of anthropogenic CO<sub>2</sub> is emitted per year, mainly from combustions of fossil fuels. The emissions of CO<sub>2</sub> into the atmosphere play an important role in global warming and lead to key environmental problems. Interestingly, enhanced oil recovery (EOR) methods have been

employed for CO<sub>2</sub> storage and improving oil recovery. For example, in 2019, CO<sub>2</sub>-EOR delivered about 2.5% of the United States crude oil supply. Traditionally in the United States, CO<sub>2</sub> from natural sources is employed for approximately 84% of CO<sub>2</sub>-EOR supply. However, CO<sub>2</sub>-EOR utilizing anthropogenic emissions would be required to attain the desired environmental benefits. Usually impurities such as CH<sub>4</sub> are present along with the CO<sub>2</sub> removed from exhaust gases of power plants and industrial processes. In this work, molecular dynamics simulations are performed to study the bulk and interfacial properties of systems containing alkanes (our model oil), CH<sub>4</sub>, and CO<sub>2</sub> under geological conditions. Linear, branched, and cyclic alkanes (C<sub>7</sub>-C<sub>19</sub>) are considered for this work. We found preferential dissolution in the alkane-rich phase and accumulation in the interfacial region of CO<sub>2</sub> from the CH<sub>4</sub>/CO<sub>2</sub> mixture. The solubility of CH<sub>4</sub> and CO<sub>2</sub> generally decreased with the number of carbon atoms in the alkane molecule  $n$  and was relatively lower in the presence of cycloalkanes. The interfacial tension (IFT) values of the CO<sub>2</sub>+alkane system increased with the addition of CH<sub>4</sub> which is in good agreement with experimental results. This can be explained by the higher enrichment of the interface in CO<sub>2</sub> than CH<sub>4</sub>. These IFTs increased with  $n$  and are relatively higher in the presence of cycloalkanes. Furthermore, the simulation results were in good agreement with the theoretical calculations based on the predictive Peng-Robinson equation of state and density gradient theory.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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MS15 / 423

## CCSNet: a deep learning modeling suite for CO<sub>2</sub> storage

**Author:** Gege Wen<sup>1</sup>

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Numerical simulation is an essential tool for understanding subsurface flow in porous media problems, yet it often suffers from computational challenges due to these problems' highly non-linear governing equations, their multi-physics nature, and the need for high spatial resolutions to capture multi-scale heterogeneity. The inherent parameter uncertainties in subsurface porous media necessitate probabilistic assessments and history matching tasks, which often require prohibitively large numbers of simulation runs. To aid engineering decisions, surrogate modeling methods are proposed by developing lower-fidelity but computationally efficient models that can provide reasonably accurate results for specific tasks. Deep learning has recently shown a growing potential for subsurface flow and transport problems. Specifically, supervised learning approaches use data generated by numerical simulators to train deep learning models and have shown encouraging results for uncertainty quantification or history matching tasks. Here, we introduce the CCSNet, a general-purpose deep-learning tool that can act as an alternative to conventional numerical simulators for a class of subsurface flow in porous media problems, namely, carbon capture and storage (CCS) problems. Unlike most proxy or surrogate models, which are developed on a task basis, we demonstrate that CCSNet provides solutions to an entire class of CCS problems where CO<sub>2</sub> is injected into saline aquifers in 2d-radial systems.

CCSNet is trained with a data set that represents almost all potential variables in the problem domain, including an extensive range of reservoir conditions, fluid properties, geological attributes, rock



properties, multiphase flow properties, and injection designs. The CCSNet consists of a sequence of deep learning models to collaboratively produce salient outputs that a conventional numerical simulator can provide, including gas saturation distributions, pressure buildup, CO<sub>2</sub> dissolution, dry-out, fluid densities in gas and liquid phases, and mass balance. The dynamic change of these outputs is captured by a tailored temporal-3d convolutional neural network (CNN) architecture. The full set of outputs also allow us to evaluate how well the results satisfy the governing conservation equations without explicitly representing them in the loss function. The results are highly resolved, nearly as accurate as numerical simulation outputs, and have excellent computational efficiencies that are 10<sup>3</sup> to 10<sup>5</sup> times faster than conventional numerical simulators. For 2d-radial CO<sub>2</sub> injection problems, our results show that CCSNet can sufficiently act as an alternative to computationally intensive numerical simulators.

To illustrate the high computational efficiency of CCSNet, we applied it to the development of rigorous estimation techniques for sweep efficiency and solubility trapping based on a stochastic sampling of the problem domains. Our results show that sweep efficiencies in homogeneous reservoirs can be predicted accurately using only three variables: the Bond number, injection rate, and irreducible water saturation. Interestingly, injection depth and injection interval had little influence on sweep efficiency. Predicting solubility trapping is more complex, requiring information about the formation permeability, irreducible water saturation, pressure, temperature, Bond number, and capillary pressure curves. Simple equations are now available to estimate both of these parameters as part of site screening process.

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## COUPLING FREE FLOW AND POROUS-MEDIUM FLOW: COMPARISON OF NON-REFINED, GLOBALLY-REFINED AND LOCALLY-REFINED AXIPARALLEL FREE-FLOW GRIDS

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In a variety of technical, medical and environmental applications, free flow coupled to porous-medium flow plays a crucial role. Due to the strong mutual interaction of the flow in both regimes, complex flow fields develop in the free-flow regime [1]. This holds especially true in the case of rough porous-medium-free-flow interfaces or when pores of a pore-network [2] touch the freeflow. Those complex flow patterns contain regions which have to be resolved in more detail than others. To resolve them, we can use overall, global or local refinement.

We use a finite-volume staggered-grid discretization, to avoid spurious pressure oscillations and to obtain local conservation. In this context we compare the overall and global refinement of axiparallel grids to a quadtree local refinement method [3].

We implemented those free-flow discretizations in our open-source simulator Dumux [4], along with a monolithical coupling to the porous medium. We present a comparison of the three refinement

strategies for various test cases. Furthermore, we discuss that distorted stencils, interpolations and local truncation errors contribute to the results we get.

**Time Block Preference:**

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**Poster + / 149**

## CPG modelling in fluvial channelised systems under uncertainty

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CO<sub>2</sub>-plume geothermal (CPG) operations are considered for sufficiently permeable formations. Fluvial sedimentary reservoirs affect losses in pump energy in heat extraction from hot sedimentary aquifers (HSA). It has been shown previously that the losses for heat extraction from HSAs can be reduced by up to 10% by orienting a doublet well pair parallel to the paleo flow trend rather than orienting it in perpendicular. In this study, we examine the same orientation-dependency of geothermal heat extraction for highly fluvial CPG operations. We use multiple realisations of highly channelized domains with control over the width, number, and straightness of the channels. We investigate the physical processes involved in CPG (such as salt precipitation, porosity-permeability changes, and pressure build-up) for these realisations.

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## CT histogram-based estimation of sub-resolution porosity of sintered lunar regolith simulant

**Author:** Li Zhuang<sup>1</sup>

**Co-authors:** Chuyen Ngoc Pham<sup>2</sup>; Sun Yeom<sup>3</sup>; Young-Jae Kim<sup>3</sup>; Hyu-Soung Shin<sup>3</sup>

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### Abstract

Moon base in the not-too-distant future has been brought to the table and the abundant lunar regolith can be used for construction materials. Due to lack of water in the moon, sintering methods (e.g., solar, vacuum and microwave), are considered to manufacture lunar regolith blocks with expected strength. Microwave sintering experiments has been conducted in our laboratory using the lunar regolith simulant under different test conditions, such as temperature and soaking time. Strength of the sintered sample is significantly influenced by the porosity and microstructure homogeneity. CT scans show that the sintered lunar regolith simulant samples are mainly composed of solid (minerals), pores and a few microcracks depending on sintering conditions. In addition, most pores have very small sizes that are sub-resolution (less than 60 micrometer in this study). Pore segmentation using the threshold-based approach ran into difficulties. Therefore we employed a novel method, called statistical phase fraction (SPF) based on CT value histograms, to estimate the sub-resolution porosity. The estimated porosities of several different samples show a good agreement with measurements through helium gas pycnometer. The key parameters for the SPF method include CT values of air and pure solid, and fitting Gaussian functions to CT histograms. Parameter estimation and sensitivity analysis for the SPF method are discussed.

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### Poster + / 805

## Calcite dissolution in crude oil and formation of crystals on surface of Mica during Ageing Process

**Authors:** Keshavarzi Shirazi Mosalman Mehrbod<sup>1</sup>; Paul Luckham<sup>2</sup>; Maja Rucker<sup>None</sup>; Apostolos Georgiadis<sup>None</sup>; Fons Marcelis<sup>None</sup>

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Ageing is a common technique within the oil industry research community to mimic the conditions of crude oil reservoir. Thereby, the porous rock is exposed to crude oil at elevated pressures and temperatures. In particular, the wettability conditions established through this procedure are known to significantly influence the flow behaviour in porous rocks. In this study ageing of mineral surfaces immersed in crude oil at 70°C and 20 Atm pressure has been conducted. During this investigation two experiments were performed. One where calcite and mica were both placed in the ageing cell

in crude oil for period of one month and one where only mica was present in the cell. An atomic force microscope (AFM) was then used to study the mineral surfaces such that topographical images of the surfaces of the minerals were produced. In both cases the structure of the adsorbed deposits could be observed and it is clear that the deposits are rather different on the two minerals. In total three different crude oils were investigated in this way. Surprisingly with one of the crudes it was observed that when the mica and calcite were aged together long needle like crystals were formed on the mica surfaces but not on the calcite. Energy Dispersive X-Ray Analysis, EDX in an SEM revealed that these crystals were comprised of calcium and sulfur, and we ascribe this to gypsum formation. Mica itself is not frequently found in reservoir rocks however it has a very similar surface to that of clays which are frequently found in the reservoir. Therefore the findings presented in this study is of particular importance as crystallisation on surface of clay in reservoir would have implications in oil recovery.

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**Poster + / 179**

## **Calculation Studies on Miscibility Characteristics of the CO<sub>2</sub>/n-Hexadecane System with Presence of Water Component under Geological Conditions**

**Authors:** Xinrong Wang<sup>1</sup> ; Dongxing Du<sup>1</sup>

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Accompanying the great achievements owing to the quick development of science and high technology, the greenhouse effect and energy crisis have shown serious negative impact to human society. Aiming at solving the two problems simultaneously, the CO<sub>2</sub> Enhanced Oil Recovery (CO<sub>2</sub>-EOR) technology has attracted wide research interests. Taking CO<sub>2</sub> as the injection fluid, this technology can not only improve the oil production, but also store large amount of greenhouse gas in underground formations, thereby to fulfill the resourceful utilization as well as the geological sequestration of the greenhouse gas.

The CO<sub>2</sub> flooding process is a typical multi-component multi-phase system consisting mainly of gas, oil and water. Thermodynamic calculations have shown great advantages of low capital and time costs compared to experimental measurements of the complex system. In correspondence to the miscibility measurements in the Pendant Drop Shape Analyzer (KRUSS DSA100HP), calculation studies on the miscibility characteristics of the CO<sub>2</sub>/oil/water system in the interfacial region of the contacting phases were performed. n-Hexadecane (n-C<sub>16</sub>H<sub>34</sub>) is employed as the oil component and water is introduced into the two phase system as the dissolved component in CO<sub>2</sub>. PR-EOS with modified alpha functions and Binary Interaction Parameters (BIPs) is employed to calculate the Minimum Miscibility Pressure (MMPs) of the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system with or without water presence at three temperatures of 40.3°C, 55.4 °C and 70°C. Calculation model and the employed parameters were validated through comparison with corresponding measurements, including the observation on decreased MMPs of the CO<sub>2</sub>/H<sub>2</sub>O/n-C<sub>16</sub>H<sub>34</sub> system in comparison with the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system. In addition, parameter studies were carried out for the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system with or without water presence at different molar ratios.

Following conclusions could be obtained:

(1) With taking water saturated CO<sub>2</sub>-rich phase in the calculation procedure, the MMPs of the

CO<sub>2</sub>/H<sub>2</sub>O/n-C<sub>16</sub>H<sub>34</sub> system were obtained at three temperatures of 40.3°C, 55.4 °C and 70°C. Comparisons between the calculation and measurement results show the maximum AD less than 10 and the AAD of 7.35%, validating the calculation results as well as the calculation model and procedure. (2) Calculation results reveal the decreased MMPs of the CO<sub>2</sub>/H<sub>2</sub>O/n-C<sub>16</sub>H<sub>34</sub> system in comparison with the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system under the same temperature, which is also comply with the corresponding measurement observations.

(3) Parameter studies were carried out for the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system with or without water presence at different molar ratios under different temperatures. It is found the existence of water component could unanimously lower the MMPs of the CO<sub>2</sub>/n-C<sub>16</sub>H<sub>34</sub> system and the degree of the MMP reduction was related to the molar ratio of CO<sub>2</sub>. It is observed that, the higher the molar ratio of CO<sub>2</sub> in the system, the larger MMP deviation between CO<sub>2</sub>/C<sub>16</sub>H<sub>34</sub> system and CO<sub>2</sub>/H<sub>2</sub>O/C<sub>16</sub>H<sub>34</sub> system. It is expected the research work could make substantial contributions to help the design of CO<sub>2</sub> EOR and greenhouse geological storage processes in the field applications.

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MS6-A / 574

## Calculation of relative permeabilities for two-phase flows in highly permeable porous media: direct calculation vs. closure problems

**Authors:** Maxime Cochenec<sup>1</sup> ; Hossein Davarzani<sup>1</sup> ; Yohan Davit<sup>2</sup> ; Stéfan Colombano<sup>3</sup> ; Ioannis Ignatiadis<sup>1</sup> ; Michel Quintard<sup>2</sup>

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Recent work shows that fluid-fluid interactions should be included in the macroscopic description of two-phase flows, at least for highly permeable porous media. Upscaling of pore-scale equations for momentum transport leads to macroscopic equations with a mobility matrix involving four relative permeability terms. Diagonal terms are standard and extra-diagonal, also called cross-terms, account for fluid-fluid interactions. Although the theoretical upscaling is known for some cases (e.g. concentric-annular flow in tube), the determination of the full matrix, either experimentally [1,2] or numerically [3,4], has proved very difficult. One approach consists in solving the closure problems derived from upscaling to compute the four relative permeabilities [5]. However, the closure problems rely on strong assumptions and miss some of the key physical ingredients of the two-phase flow problem.

Here, we show that a technique based on variations of a body force allows us to precisely calculate these four relative permeabilities. The idea is to alternatively apply a slightly different body force to each fluid to calculate coupling terms. In this model, we maintained a constant phase distribution and saturation, a condition which is not always fulfilled in the literature. We show, in a simple 2D geometry, that the results from the closure problems fail because the boundary conditions at the interface between the fluids do not allow to account for the complexity of the flow, e.g. by neglecting important viscous dissipation zone. Therefore, we propose to modify the fluid-fluid boundary conditions for velocity in the closure problem to account for these dissipation zones. We further find that the non-diagonal relative permeability terms are not negligible. This fact is in agreement with previous work for film flow in simple 2D cells with a solid obstacle.

The proposed numerical method can be used to calculate the relative permeability, including cross terms. The main advantage of the modified closure problem is that its computation time is low. This technique may be a good alternative in some cases (e.g. for low capillary number). We anticipate that the elements brought in this work on the choice of the body force variations could serve as a basis for the calculation of relative permeabilities in more complex geometries.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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**Poster + / 609**

## Capillary imbibition dynamics under various solid–liquid interactions: A molecular dynamics study

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**Co-authors:** Zhibing Yang<sup>1</sup> ; Ran Hu<sup>1</sup> ; Yi-Feng Chen<sup>1</sup>

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Capillary imbibition, i.e. the spontaneous flow of a liquid into fine pores and cracks without the assistance of external forces such as gravity, is universal and critically important in many natural processes and industrial applications. On the nanoscale, the intensity of solid–liquid interactions ( $\epsilon_{S-L}$ ), which controls the wettability of the capillary walls, plays a critical role and directly affects the imbibition rate, the shape of the meniscus, the evolution of the dynamic contact angle, and even the viscosity of the confined fluid. Here we use molecular dynamics simulations to systematically investigate how  $\epsilon_{S-L}$  influences the capillary imbibition dynamics in a nanochannel. We quantify the relationship between the equilibrium contact angles and  $\epsilon_{S-L}$ , and find that the cosine of equilibrium contact angle increases linearly with  $\epsilon_{S-L}$ . Subsequently, we investigate the capillary dynamics under a wide range of solid–liquid interactions. We show that the capillary rate increases with  $\epsilon_{S-L}$ , while an overlarge  $\epsilon_{S-L}$  may hinder the further growth of the imbibition rate. We also characterize the evolution of the dynamic contact angle, imbibition rate, imbibition length. The findings in this work could provide new insights into the capillary imbibition dynamics on the nanoscale.

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## Capillary pumping: a transport mechanism in partially wet porous networks

**Author:** Joachim Falck Brodin<sup>1</sup>

**Co-authors:** Marcel Moura<sup>2</sup>; Knut Jorgen Maloy<sup>3</sup>; Per Arne Rikvold<sup>4</sup>

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We present preliminary results from experiments investigating fluid transport in partially wet porous media. Our experiments mimic the natural processes that happen for example when a water-soluble pollutant is spilled on humid soil and is gradually transported inside the network, following the gradient of the matrix potential. We utilize a synthetic quasi 2D matrix of glass beads in a Hele-Shaw cell. The cell is prepared with a controlled degree of clear water saturation which in turn is put in contact with a droplet of dyed water. The cell is transparent and resting horizontally on a light box, with a camera monitoring from above. Through imaging and image analysis we have quantified the spreading efficiency of the networks and showed how this efficiency depends on the initial water saturation in the sample. Our observations indicate the existence of a critical soil water saturation, for which the spreading process attains maximum range. Our findings bring consequences of relevance to the understanding of pollution dispersion in natural soils and the associated mitigation and remediation strategies.

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MS5 / 771

## Capsule-based biomimetic regulating technique of MICP and its application for soil reinforcement

**Author:** Alexandra Clarà Saracho<sup>1</sup>

**Co-authors:** Lorenzo Lucherini<sup>1</sup>; Dimitrios Terzis<sup>1</sup>; Lyesse Laloui<sup>1</sup>

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Microbial induced calcium carbonate (CaCO<sub>3</sub>) precipitation (MICP) not only plays a dominant role in the carbon cycle but is also a promising technology to create living building materials. However, the short shelf-life, lack of spatial control and limited scalability have hindered their use commercially. To tackle these shortcomings, we herein present a capsule-based biomimetic regulating technique of MICP. The ureolytic bacterium *Sporosarcina pasteurii* is immobilised in hydrogel droplets via extrusion and calcium ion cross-linking, and its controlled release is achieved through competitive displacement of the calcium ions between the polymer and the peptides in the yeast extract. This highlights, for the first time, the potential to program the release of the biochemical machinery of MICP, with the recognition of a component that is inherently specific to the solution used to promote bacterial growth. Our concept, integrating MICP with soft materials for controlled dynamic

metabolic response and calcium carbonate mineral microstructure, is finally demonstrated in soil specimens to showcase its applicability in the context of soil reinforcement. This platform technology constitutes a step change in the design of functional living building materials that can sense, respond, and heal.

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MS21 / 610

## Cell-scale haemodynamics and transport in canonical disordered porous media: numerical simulation and microfluidic experiments

**Authors:** Qi Zhou<sup>1</sup> ; Kerstin Schirrmann<sup>2</sup> ; Igor L. Chernyavsky<sup>3</sup> ; Anne Juel<sup>2</sup> ; Oliver E. Jensen<sup>4</sup> ; Miguel O. Bernabeu<sup>5</sup> ; Timm Krüger<sup>1</sup>

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Key words: porous media, haemodynamics, heterogeneity, modelling, microfluidics

### Introduction

While extensive research has been devoted to fluid flows through porous media with comprehensive theories established ranging from pore-scale to field-scale (single-phase or multiphase, inertial or non-inertial, Newtonian or non-Newtonian, Darcy or non-Darcy), the underlying mechanisms for the flow and transport of blood and nutrients in biological organs/tissues such as the highly porous human placenta are still unclear [1]. As the size of flow channels within these systems becomes comparable with that of a red blood cell (RBC, about 8  $\mu\text{m}$  in diameter), the particulate character of blood gives rise to complex nonlinearity by introducing spatiotemporal heterogeneities that require microscopic interrogation. In this work, we aim to characterise the microscopic blood flow within canonical porous media consisting of disordered pillar arrays. Both flow simulations at the microscale and corroborating experiments in a microfluidic analogue will be presented.

### Methods

The porous media models are constructed by introducing different levels of disorder to regular obstacle arrays arranged on a square grid. Using the lattice Boltzmann and immersed boundary methods [2, 3], we simulate blood flow through the disordered geometry as a suspension of deformable RBCs in plasma. The volume fraction of RBCs (known as haematocrit) simulated is in the range of 20%-30%. In parallel with the numerical model, a microfluidic analogue with equivalent conditions (e.g. confinement ratio and capillary number) is designed and fabricated, in which flow experiments are performed with monodisperse capsules (about 250  $\mu\text{m}$  in diameter) that imitate the properties of RBCs.

### Results

Our results show an intricate interplay of structural disorder, rheological uncertainty, and time-dependent effects on the localisation of RBCs within a porous medium, which is highly heteroge-



neous presenting preferential paths subject to the “channelling effect” [4, 5] as well as emerging cell occlusion. We report for the first time the effect of incremental disorder within the porous media on the overall hydrodynamic resistance of the cellular blood flowing through, which markedly increases as the level of disorder introduced into the system, whereas in the Newtonian counterpart (for which only plasma is infused) a larger degree of disorder has a much weaker effect.

### Discussion

The role of RBCs in the intervillous space within the human placenta is multifold. On the one hand, the RBCs facilitate the transport of oxygen, CO<sub>2</sub> and other solutes. On the other hand, RBCs’ localisation can significantly affect the flow patterns in the porous media, which are not well-captured by Darcy’s law. Thus, more generalised constitutive relationships need to be derived based on cross-validation of simulations and experiments to bridge microscopic characterisation and organ-level modelling.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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## Characterising multi-domain porous structure of the human placenta by synchrotron X-ray micro-tomography

**Authors:** Win M. Tun<sup>1</sup> ; Gowsihan Poologasundarampillai<sup>2</sup> ; Helen Bischof<sup>3</sup> ; Gareth Nye<sup>4</sup> ; Oliver N. F. King<sup>1</sup> ; Mark Basham<sup>5</sup> ; Yasuaki Tokudome<sup>6</sup> ; Rohan M. Lewis<sup>7</sup> ; Edward D. Johnstone<sup>3</sup> ; Paul Brownbill<sup>3</sup> ; Michele Darrow<sup>8</sup> ; Igor L. Chernyavsky<sup>9</sup>

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Multi-scale structural assessment of biological soft tissue is challenging but essential to gain insight into structure-function relationships of tissues and organs [1-4]. The human placenta is one of the most complex vascular organs of the human body. It is an exchange organ with a large surface area

of the feto-maternal interface packed in a relatively small volume. The human placenta has the total length of the feto-placental vascular network of over 550 km, and its tightly integrated structural constituents span the spatial range from  $\sim 10^{-6}$  to  $10^{-1}$  m [1,2].

Using the human placenta as an example, this study brings together advanced sample preparation protocols, three-dimensional imaging and modelling to provide the first massively multi-scale information that enables detailed morphological and functional analyses of multiple placental domains [5].

We employ machine learning-based segmentation techniques for robust and efficient decomposition of maternal and fetal micro-domains which bridge almost four orders of magnitude (from microns to centimetres). Spatial statistical analysis and flow simulations are performed on the feto-placental vascular network and associated intervillous porous space, and we validate the results against other modalities, such as traditional 2D stereology and in-vivo magnetic resonance imaging. Finally, we quantify the scale-dependent error in morphological metrics of heterogeneous placental tissue, estimating the minimal tissue scale needed in extracting meaningful biological data.

The developed protocol is beneficial for high-throughput investigation of structure-function relationships in both normal and diseased placentas, allowing us to optimise therapeutic approaches for pathological pregnancies. In addition, the methodology presented is applicable in characterisation of tissue architecture and physiological behaviours of other complex organs with similarity to the placenta, where there are complex fluidic / exchanger systems, such as represented by the kidney, lung, lymphatics, spleen and the central nervous system.

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**Poster + / 640**

## Characterization of microbial distribution of packaging material processes over a production cycle

**Author:** Stephanie Maitz<sup>1</sup>

**Co-authors:** Paul Jakob Schmid<sup>1</sup> ; Clemens Kittinger<sup>1</sup>

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Microbial growth and biofilm formation are to be expected in many water circulation systems as it is also the case in production facilities for packaging materials. Consequently, these factors can impair the production, may lead to increased downtime and higher costs. Therefore, this study focuses on the determination of microbial composition of different phases involved in the manufacturing process of varying packaging materials. These phases comprise the process water, the porous packaging material itself, and biofilms. Illumina next-generation sequencing was used in order to identify composition on genus level and possible key organisms.

In terms of biodiversity, biofilm samples feature a high diversity of microorganisms with up to twenty different microbial classes per investigated sample.

Process water samples showed a reduced diversity; the classes found are consistent with the classes present in the biofilm samples.

Main classes of Gammaproteobacteria, Deinococci, Bacteroidia, Bacilli, Alphaproteobacteria and Clostridia were detected. Moreover, the biodiversity depended on cleaning procedures of the production facility. In all samples, the classes of Gammaproteobacteria, Deinococci, Bacteroidia, Bacilli and Alphaproteobacteria were detected over time of sampling. After one cleaning step an increased diversity of microorganisms was observed, which was reduced again until the next cleaning step.

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MS6-B / 288

## Characterization of wettability control on dynamics of two phase flow in natural porous media

**Authors:** Sahar Bakhshian<sup>1</sup> ; Harris Sajjad Rabbani<sup>2</sup> ; Nima Shokri<sup>3</sup>

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Leveraging high-fidelity lattice Boltzmann simulations (1,2) combined with analytical modeling, we investigate the interplay of surface wettability, small-scale heterogeneity of the pore geometry, and mobility conditions influencing the characteristics of immiscible two-phase fluid displacement in natural porous media (3). We present a detailed pore-scale analysis of flow regimes occurring during favorable ( $M > 1$ ) and unfavorable ( $M < 1$ ) displacement conditions in a rock sample of Tuscaloosa sandstone under a wide range of wettability ( $25^\circ < \theta < 175^\circ$ ). As manifested by the saturation profile of invading fluid, we distinguished a transition of invasion morphology from fingering to compact (stable) displacement as the wetting condition varies from drainage to strong imbibition under both favorable and unfavorable mobility conditions. It becomes evident that the appearance of corner-flow plays a key role in the emergence of the transition zone in the displacement patterns. Furthermore, the corner-flow active zone is found to be mainly concentrated ahead of the primary invasion front and it is heterogeneously distributed in the pore space, preferentially hosted by small pores. It is found that the heterogeneous distribution of corner-flow events does not necessarily impose an adverse effect on the recovery of the defending fluid, as the maximum recovery efficiency is observed under the strong imbibition condition, where the corner flow is prevalent. In addition to numerical simulations, we derived an analytical model that can forecast the saturation profile of fluids as a function of wettability under different boundary conditions. The analytical model showed a reasonable agreement with the numerical results and can be a useful diagnostic tool for optimizing the displacement process in porous media (4).

**Key words:** Porous media, Heterogeneity, Two-phase flow, Wettability, Lattice Boltzmann modeling

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#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS4 / 478

## Clay settling in fresh and salt water: new dynamic X-ray micro-CT insights

**Author:** Wesley De Boever<sup>1</sup>

**Co-authors:** Jan Dewanckele<sup>1</sup>; Andreas Griebner<sup>2</sup>; Yanhong Wang<sup>3</sup>; Fangli Meng<sup>4</sup>

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Complex clay systems are present all over the world and play a major role in many applications. In sedimentation processes for example, it is known that the settlement of clay particles is slow when they are exposed to fresh water. However, when exposed to salt water, the dynamics of the particles drastically change. The clay particles flocculate and results in a separation of an almost pure water section on top and a water and clay suspension below. This flocculation process starts within minutes with a formation of a clear concentration front. Once the flocculation is finished, a dense mass of clay (chemical bounded with positively charged salt ions) remains. On the other hand, if this dense mass of clay (also referred as salt rich glaciomarine salts), is uplifted and no longer exposed to saltwater, rainwater can infiltrate and diffuse the salts out of the clay. In some occasions this may result in massive landslides as the freshwater destabilizes the clay aggregate structures.

As another example, clay minerals such as bentonite are also widely present in various ore bodies, mainly as gangue minerals. For mining industries, the processing of those ore bodies is very challenging as the presence of clay results in poor flotation performance. The coating of the clay on the valuable ore minerals reduces the recovery of those minerals. The presence and addition of salt ions in water may have a significant effect on the slime coatings (Chen and Peng, 2018) and pulp rheology (Huang et al., 2020) enhancing for example chalcopyrite recovery (Jeldres et al., 2019).

In order to better understand the above-described complex interactions of clay, salts and water, an in situ experiment was performed in a TESCAN CoreTOM, enabling 4D visualization and better understanding of the clay behaviour. By using high speed X-ray micro-CT (dynamic CT) we were able to visualize the flocculation pattern, in three dimensions as a function of time, of bentonite clay in fresh water, NaCl solution, and KCl solution. In this study, 8 g bentonite was mixed with 2 g chalcopyrite in 1) 50 mL DI water, 2) 50 ml DI water + 1mol/L NaCl and 3) 50 ml DI water + 1mol/L KCl. The suspension was stirred for 15 min before subsampling. Micro-ct was acquired using scans with a continuous speed of 5.8 sec/ rotation (0°-360°) and a voxel size of 15 µm. In total 100 uninterrupted rotations were acquired with 400 projections each. Both temporal and spatial resolution was sufficient to visualize and analyse the dynamics in three dimensions showing clear differences between the systems. Motions of particles were analysed using the Software GeoDict.

Along with playing a critical role in soil stability and mining applications, bentonite is a widely used clay in many industrial products such as paints, ceramics, drilling fluids, etc. Although commonly used, the bentonite-water systems are not yet fully understood. The authors hope that these initial experiments may open doors towards many other applications and a better understanding of these, and similar, dynamic interactions.

#### **Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## **Coal Relative Permeability Measurements Using Lab-on-a-chip Method**

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Coalbed methane (CBM) plays a critical role in transiting the global energy supply from fossil fuel to renewables in the next 30 years. To understand and forecast CBM reservoir performance, coal relative permeability curves are needed as a key input parameter in reservoir simulators. Currently the relative permeability curves are normally measured using steady-state method at the laboratory conditions, where each effective flow capability of the coal core is then plotted against the corresponding water saturation. Field experience has constantly showed that the predicted results based on the curves from the steady-state method often overestimate field production.

In this work, the lab-on-a-chip (LOC) method was adopted to measure the evolution of relative permeability under controllable and repeatable conditions, and meanwhile to visualize water-gas two-phase in microchannels to gain critical flow information that conventional laboratory measurements are unable to offer. As the start, a single-channel microfluidics made of PDMS was first fabricated with a dimension of  $100 \times 100 \mu\text{m}$  (width by depth) and 24 mm in length. A number of tests were then conducted, including (i) the advancing contact angles of water with different wettability properties and the static contact angle to water and methane gas, (ii) similar to steady-state method, a series of injection tests with different gas-water volume ratios were conducted. Factors such as the flow velocity of each phase, the characteristics of flow field, and flow pressure of each phase, were also monitored; and (iii) the second step was repeated with different water wettability and injection rates. The results show that the shape of water relative permeability from microfluidics tests is similar to that from conventional laboratory testing, but the gas relative permeability curve is very different between the two methods. The water relative permeability is 30 times lower than that predicted by Chima's model, and the gas relative permeability is even lower, 160 times. One reason, from our direct experimental observations, is that gas and water form discontinuous plug flow inside the microchannel and the interaction between the two phases along water-wetting surface significantly reduces gas flow capacity.

In addition, our results show that relative permeability values increase with injection rates and wettability, ranging from 10% to 20%. This work offers some interesting results that have rarely been captured and analyzed in core flooding measurements, and meanwhile the differences in relative permeability curves indicate that the data uncertainty associated with the steady-state method may be worth re-assessing.

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MS6-A / 492

## Coffee is for drinking, tea is for porous media science: intermittent burst dynamics in slow drainage experiments in porous media

**Authors:** Marcel Moura<sup>1</sup> ; Knut Jørgen Måløy<sup>1</sup> ; Eirik Flekkøy<sup>1</sup> ; Renaud Toussaint<sup>2</sup>

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We start with a very simple experiment that you can reproduce in your own kitchen. Being stuck in this home office business does not mean we have to stop with the experimental activity! Make yourself some tea. No fancy loose-leaf tea, just the regular teabag from the store around the corner. Place the teabag in a cup and after you are happy with the tea's strength, remove the bag and place it on top of a napkin (preferably on a plate or something to control the mess in your kitchen). You can now get rid of tea, the teabag is all that matters, that's where the porous medium is. Watch it closely: you will see that as the napkin gets wet, pockets of air suddenly enter the void spaces between the tea leaves, in a very abrupt fashion. This kind of intermittent invasion dynamics is common to all types of drainage experiments in porous media. We have studied this behavior experimentally using artificial micromodels that (unlike the tea), are completely transparent, thus allowing us to visually track the whole invasion dynamics. We have measured the pressure fluctuations resulting from the intermittent burst activity, and showed how different boundary conditions (controlled imposed pressure vs. controlled withdrawal rate) lead to very different pressure signatures. We have shown how statistical signatures of the pressure fluctuations can encode important information about the porous medium and the liquids involved.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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**Poster + / 183**

## **Comparative study on oil recovery efficiencies of ScCO<sub>2</sub> and N<sub>2</sub> injection processes in tight cores**

**Authors:** Chaofan Li<sup>1</sup> ; Dongxing Du<sup>1</sup>

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Under the contradiction of the fast depletion of oil production from conventional reservoirs and the increasing energy demand, unconventional oil and gas reservoirs, such as tight oil, tight gas and shale gas, have played more and more important role in the world's energy supply. Gas injection process has contribute one of the most efficient oil recovery methods on tight oil recovery practices. To reveal the oil recovery mechanisms and the field applicability of gas injection technique, Super-critical CO<sub>2</sub> (ScCO<sub>2</sub>) and N<sub>2</sub> injection process in oil saturated tight cores were comparatively studied in this paper.

The Bentheimer sandstones with different permeability of 0.02mD, 0.5mD and 5.6mD were employed as the tight sample cores, and the gas injection processes were performed under two backpressure conditions of 15MPa and 25MPa at temperature of 50°C. Through quantitative comparisons of the oil recovery factor and the displacement pressure difference parameters, the oil recovery efficiency and mechanisms of ScCO<sub>2</sub> and N<sub>2</sub> flooding processes has been comprehensively investigated.

The experimental results show that,

1)The recovery efficiency of ScCO<sub>2</sub> injection process increases with the increase of core permeability and system pressure. Under the system back pressure of 15MPa, the oil recovery rate increases from 59% to 91% with the increase of permeability. At the elevated system pressure of 25MPa, the recovery efficiency of CO<sub>2</sub> displacement could reach the level of 84%~92%. Larger pore-throat sizes in the higher permeable cores as well as the higher miscibility content at higher pressures could contribute to above experimental observations.

2)The recovery efficiency of N<sub>2</sub> injection process increases with the increase of core permeability and system pressure as well. Under the system back pressure of 15MPa, the oil recovery rate increases from 26% to 40% with the increase of permeability. At the elevated system pressure of 25MPa, the recovery efficiency of N<sub>2</sub> displacement could approach to 21%~52%. Large pore-throat sizes in the higher permeable cores as well as the lower interfacial tension (IFT) between oil and gas phase at higher pressures could contribute to above experimental observations.

3)Under the same experimental conditions, ScCO<sub>2</sub> injection shows unanimously and remarkably higher oil recovery rate compared with the N<sub>2</sub> injection process, indicating the advantage and the potential application of the miscible ScCO<sub>2</sub> injection process on tight oil reservoir development practices.

It is expected this work could help the reservoir applicability investigations of the gas injection processes based on the oil recovery effects as well as the in-depth understanding of the mechanisms of ScCO<sub>2</sub> and N<sub>2</sub> displacement in tight oil reservoirs.

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Poster + / 256

**Comparision Modified Method of Peng-Robinson Equation of State in the Process of Gas Injection of Nanopores****Author:** yuan zheng wang<sup>1</sup>**Co-authors:** ☒☒; ☒☒<sup>1</sup> CHINA UNIVERSITY OF PETROLEUM (beijing)**Corresponding Authors:** caorenyi@163.com, 1205161792@qq.com, mamingupc@163.com

With the development of large quantities of gas injection in shale and tight reservoirs, the multi-phase behavior in nanoscale pores before and after gas injection has gradually attracted people's attention. A large number of published literature have shown that due to wall adsorption and capillary force, the phase behavior of confined fluid in micro and nano pores is significantly different from that of conventional reservoirs, such as phase transformation hysteresis. The existing EOS equation, especially the PR-EOS method for the calculation of gas-liquid equilibrium, has been unable to accurately describe the change of gas-fluid phase state in nanopores. Therefore, it is necessary to modify the EOS equation according to the relevant terms introduced in the phase state mechanism of corresponding nano pores or combining with other methods. Our discussion focuses on three kinds of correction methods for phase state calculation in nanoscale pores, including: correction of gravitational phase and volume parameters in the equation of state; The capillary force and critical parameters in micro-nano pore channels were considered; Engineering Density Functional Theory (DFT) is combined with equations of state. Although the above methods in the literature are in order to improve the EOS model in the prediction of phase behavior change in a nanoscale pore precision for the result, but in the case of a given component simulated calculation, in the process of gas injection, the component concentration changing, each part of the existing EOS correction method adaptability to variable components is unknown, and they lack of contact with each other between various correction method. This discussion through the three kinds of PR - EOS correction method of micro/nano pores in the process of gas injection gas - liquid phase change contrast the actual situation of deviation rate, consider in the process of high temperature and high pressure gas injection with different pore scale, selection and analysis of the influence of key parameters on the phase behavior change and its sensitivity, finially,we can obtained gas fluid EOS correction method of the accuracy and applicability after gas injection in the micro/nano pores. The results show that the three nano-scale pores phase state correction methods can reflect the phase state change better to a certain extent. Considering the change of composition, the changes of capillary force and critical parameters in micro and nano pores are more concise and the adjustable parameter range is larger. The fitting results can better reflect the changes of fluid phase state in micro and nano pores. The other two methods can clearly consider the intermolecular and fluid-surface interaction forces and can explain the restricted fluid phase behavior in micro and nano pores from the molecular perspective, but the calculation process involves large-scale calculation and is relatively complex.

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**Student Poster Award:**

**Poster + / 802**

## Comparison and Reduction of the Chemical Kinetic Mechanisms Proposed for Thermal Partial Oxidation of Methane (TPOX) in Porous Media

**Authors:** Farzam Fotovat<sup>1</sup> ; Mehrnaz Rahimpour<sup>2</sup>

<sup>1</sup> Sharif University of Technology

<sup>2</sup> Sharif University of Technology

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The effectiveness and reducibility of the methane combustion kinetic mechanisms were examined for the TPOX process in a porous medium. To this end, TPOX was successfully simulated using ANSYS CHEMKIN-Pro through a reactor network model composed of perfectly stirred and honeycomb-monolith reactors. The efficacy of six chemical kinetic mechanisms was compared for the equivalence ratios (ERs) ranging from 2.4 to 2.6 with a constant thermal load of 1540 kW/m<sup>2</sup>. This comparison revealed that Konnov was the most successful mechanism in the prediction of the H<sub>2</sub> and CO mole fractions. This mechanism along with the GRI-3.0 and USC-Mech 2.0 mechanisms were then reduced by the direct relation graph with error propagation (DRGEPSA) followed by the full species sensitivity analysis (FSSA). This approach reduced the number of species from 119 to 29 for the Konnov mechanism, from 53 to 23 for the GRI 3.0 mechanism, and from 111 to 34 for the USC-Mech 2.0 mechanism.

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**Poster + / 749**

## Comparison of Response Surface and Artificial Neural Network Model for Relative Permeability using Saturation and Phase Connectivity

**Author:** Hanif F. Yoga<sup>1</sup>

**Co-authors:** Prakash Purswani<sup>1</sup> ; Russell T. Johns<sup>1</sup>

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Hysteresis in transport properties such as relative permeability remains a challenge for reservoir simulations of multiphase processes such as CO<sub>2</sub> sequestration as well as chemical enhanced oil recovery (EOR). Modeling relative permeabilities as a state function with the knowledge of the parameters that affect relative permeabilities has shown promise in mitigating hysteresis.

In this research, we advance the development of the relative permeability equation-of-state ( $kr$ -EOS) by considering quadratic and cubic polynomial forms for relative permeability ( $kr$ ) in the space of state parameters, namely, phase saturation ( $S$ ) and phase Euler connectivity ( $\chi^*$ ). We maintain other state parameters, such as wettability, pore structure, and capillary number, to be constant. We consider numerical data sets of nonwetting phase  $kr$ ,  $S$ , and  $\chi^*$  for two different contact angles in the water-wet regime using pore-network modeling (PNM). These data sets include multiple sets of primary drainage, imbibition, and secondary drainage scanning curves. We constrain the polynomial functions of  $kr$  in the physical  $\chi^*$ - $S$  space traversed by the PNM data. Next, we use linear regression to fit the models to the numerical data and analyze the behavior of the  $kr$  response as well as the partial derivatives of  $kr$  in the  $\chi^*$ - $S$  space. These are also compared to the numerically calculated  $kr$  partials. A comparison of the tradeoffs between the quadratic versus the cubic response is presented. Furthermore, using these regression models, we extend the EOS approach and couple with machine learning algorithms. We develop a physics-based Artificial Neural Network (ANN) algorithm to provide a practical estimate of the values and paths of  $kr$ , using the numerical data sets and polynomial variables as the designated inputs. A comparison of the accuracy between the polynomial functions and the ANN model is presented.

Our results show that a cubic or higher-order response function is needed to capture reasonably well the behavior of  $kr$  over the entire physical  $\chi^*$ - $S$  space for different cycles of injections. This is because only a cubic or higher-order polynomial can capture the complex behavior of the locus where relative permeability is zero (the locus of residual saturation and residual phase connectivity). The cubic response also allows us to capture the behavior of the  $kr$  partial derivatives as defined by the EOS in the  $\chi^*$ - $S$  space. Lastly, the machine learning framework helps implement a hybrid approach which incorporates a data-driven model while still honoring the physics-driven polynomial responses. This method provides further improvement compared to both the response surface approach and conventional estimation methods of  $kr$ . The described methodology and functions will aid in modeling complex hysteresis that occur in both CO<sub>2</sub> storage and in EOR processes.

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MS3 / 665

## Comparison of mechanical and hydro-mechanical models for rough fracture closure

**Author:** Amanzhol Kubeyev<sup>None</sup>

**Co-authors:** Kevin Bisdom<sup>1</sup> ; Niko Kampman<sup>1</sup> ; Florian Doster

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Flow in fractured porous media is in part controlled by the fluid pressure within the fracture, which is typically modelled by assuming planar fracture surfaces. However, experimental data has shown that the geometry of non-planar, i.e. rough fracture surfaces impacts both permeability and its dependency on stress. Various (semi-)analytical and numerical methods have been developed to describe this stress-permeability relationship in rough fractures. This paper aims to compare two methods and analyze the suitability for a particular purpose: a) numerical contact mechanics based

fracture closure using Virtual Element Method connected to Stokes flow solver and b) analytical McDermott closure connected to 3D Darcy flow solver. We investigate the mechanical and hydro-mechanical evolution of a rough fracture with synthetically created and natural mudrock surfaces. The roughness is represented by heights profiles and parametrized by the fractal dimension and by the root mean square of heights. Simulation is carried by taking 2D cross-sections from the 3D surface and compared against the McDermott model. Results of two approaches compare well for the stress-aperture and stress-permeability relationships, and McDermott model can be used for general purposes. However, the numerical method offers more flexibility for more specific modelling such as modelling exact fracture roughness, implementation of nonlinearities in the material or failure. Besides, the normalized aperture vs. the number of contacts relationships, which is related to the fracture roughness, were proposed for the use in McDermott.

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MS7 / 430

## Compositional modeling in porous medium using iterative IM-PEC scheme and constant volume-temperature flash

**Authors:** Tomáš Smejkal<sup>None</sup> ; Jiří Mikyška<sup>None</sup>

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In this contribution, we present a new numerical solution of a two-phase compressible Darcy's flow of a multi-component mixture in a porous medium. The mathematical model consists of mass conservation equation of each component, extended Darcy's law for each phase, and an appropriate set of the initial and boundary conditions. The phase split is computed using the constant temperature-volume flash (known as  $VTN$ -specification) [1]. The transport equations are solved numerically using the mixed-hybrid finite element method and a novel iterative IMPEC scheme [2]. We provide examples showing the performance of the numerical scheme.

**Time Block Preference:**

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MS12 / 441

## Computational analysis of Single- and Two-Phase Flow with Poroelasticity

**Author:** Maria Warren<sup>1</sup>

**Co-authors:** Hongkyu Yoon <sup>1</sup> ; Mario J. Martinez <sup>1</sup> ; Alex Kucala <sup>1</sup> ; James E. Bean <sup>1</sup>

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Coupled poromechanics involving single and multiphase flow during carbon sequestration, geothermal recovery, and waste disposal requires accurate numerical modeling of coupled processes in porous media. Over the past decade, iterative coupling schemes have been leveraged to model these coupled poroelastic problems. Specifically, the fixed stress scheme has been successfully used to solve poromechanics problems that involve both fluid and solid mechanics. In this work, two methods for implementation of the fixed stress scheme into the Sandia Sierra Multiphysics toolkit [1-3] are compared: one through an existing thermal/fluid mechanics module (ARIA) and the other through integration of the ARIA with the Sierra solid mechanics (SM) module. First, the fully coupled method of ARIA was compared with analytical solutions for poroelastic problems such as one-dimensional (Terzaghi), two-dimensional (Mandel), and three-dimensional (Cryer Sphere) problems. Model comparison shows that the fully coupled method in ARIA accurately match analytical solutions for all three problems. Second, the fixed stress schemes implemented in the Sierra SM were evaluated against the fully coupled numerical model. This work provides a unique comparison of the accuracy and computational demand for two implementations of the fixed stress scheme (ARIA and ARIA with SM) over a wide range of porous media properties. This research also shows that the fixed-stress scheme decreases early oscillations in pore pressure for first-order, linearly interpolated finite elements, versus the fully coupled model. Then, stability of the fixed stress scheme is further investigated by evaluating two different GMRES (generalized minimum residual method) solvers available in Sierra Multiphysics toolkit. Third, the fixed stress scheme is expanded into multi-phase flow problem where effective pore pressure is calculated in two different ways, including saturation weighted method and thermodynamic-based method. Through modeling of a water-air system, the accuracy of two-phase flow with the fixed stress scheme and calculation of effective pore pressure is evaluated. This work advances current single- and two-phase flow modeling techniques through a detailed description of fixed stress scheme implementation within multi-physics solvers.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525

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**Poster + / 608**

## **Computational modeling based on decomposition methods applied to polymer flooding in oil reservoir**

**Authors:** Rodrigo Silva Tavares<sup>1</sup> ; Renatha Batista dos Santos<sup>1</sup> ; Sidarta Araujo de Lima<sup>1</sup> ; Adriano dos Santos<sup>1</sup> ; Viviane Klein<sup>1</sup>

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Polymer flooding is an enhanced oil recovery technique applied to reduce mobility ratio and improve sweep efficiency [7]. In addition, polymer solutions can be used as relative permeability modifiers (RPM) in order to increase the recovery factor due to flow diversion [1]. In the applications mentioned above, high viscosity and polymer retention (mechanical retention and adsorption) may cause injectivity problems in cases where there are limitations on injection pressure [7]. In the techniques mentioned above, accurately modeling the coupling between the near-well region and the rest of the reservoir phenomena in different spatial and temporal scales is essential. For instance, a local spatial and temporal mesh refinement is necessary near the well to capture the formation damage and non-Newtonian behavior. However, refining the entire reservoir is impractical due to the high computational cost [5]. Therefore, an alternative to efficiently couple these regions is to apply a space-time domain decomposition technique. The main idea is to split the reservoir domain into subdomains with appropriate space-time refinement, taking advantage of the parallel computational architecture to reduce computational cost. This work aims to deduce an innovative mathematical and computational model for polymer flooding in oil reservoirs based on domain decomposition techniques to efficiently couple the near-well region and the reservoir. The governing two-phase flow equations consist of Darcy's law and mass balance for fluid (oil and water) together with the transport equation for the polymer movement in the aqueous phase [7]. Additional closure equations are applied to describe adsorption, mechanical retention, formation damage, and the non-Newtonian pseudoplastic behavior. For the computational model, Darcy's law and total mass balance are discretized by applying the mixed finite element method [3]. Moreover, the aqueous phase and polymer transport equations are approximated using the central upwind finite volume scheme [4]. To the domain decomposition method, we consider the reservoir domain partitioned into nonoverlapping subdomains. Then, for the hydrodynamics equations, the mortar finite element method is applied to ensure continuity of pressure and fluxes across the interfaces [2]. For the transport equations, due to the hyperbolic PDE nature, the explicit finite volume method is applied assuming Dirichlet interface conditions to compute the solution for saturation and polymer concentration [6]. To validate the accuracy and stability of the proposed computational model, we propose some numerical simulations by comparing the discrete solutions with analytical and high-fidelity solutions. We also simulate the dependence of the injectivity and production curves with the non-Newtonian behavior, mechanical retention, and formation damage considering more general domains, such as the five-spot reservoir in the presence of perforated wells. The numerical simulations show that the proposed computational model has a low computational cost and accurately captures the solutions in several scenarios for polymer flooding in oil reservoirs.

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## Conceptual model of reactive transport incorporating with dynamic biofilm growth and multicontinuum media

**Authors:** Jingjing Wang<sup>1</sup> ; Maarten W. Saaltink<sup>1</sup> ; Jesús Carrera<sup>2</sup>

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Biofilm growth in porous media changes the hydrodynamic properties of the medium: porosity and permeability are reduced, and dispersivity increases. However, the first arrival of breakthrough curves (BTCs) is more reduced than derived from the reduction in porosity, and the BTC tail becomes heavier. These observations suggest the need of multicontinuum models (Multirate-Mass-Transfer, MRMT) that evolve dynamically with the biofilm. The MRMT model is capable of representing reactive transport in heterogeneous porous media which facilitates the simulation of localized reactions often observed within biofilms. In this work, we present a conceptual model of reactive transport with dynamic biofilm growth based on MRMT formulations. It incorporates the microbial growth according to the stoichiometry and kinetic rate laws of biological reactions. The physical, including not only porosity and permeability, but also the distribution of residence times in immobile zones, and chemical properties are updated after the reactive transport simulations at each time. This model is tested on field and laboratory data.

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## Cone beam computed tomography reconstruction for digital rock

**Authors:** Vijitha Periyasamy<sup>1</sup> ; Vishal Metri<sup>1</sup> ; Avanindra Singh<sup>1</sup> ; Ronny Hoffman<sup>2</sup> ; Kunj Tandon<sup>3</sup> ; Phaneendra K Yalavarthy<sup>4</sup> ; Jaya Prakash<sup>5</sup>

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Digital rock physics (DRP) is the derivation of rock properties from scanned volumes of core plugs [1]. The scanning modalities include 2D-based techniques such as light sheet microscopy, scanning electron microscopy and confocal microscopy, which gives slice-wise information of the rock, and 3D-based techniques such as clinical x-ray tomography, cone beam computed tomography (CBCT), and magnetic resonance imaging, which results in volumetric information of the rock. CBCT imaging, widely used for pore scale studies, provides a relatively high resolution (1 to 4 micrometers) in a reasonable time frame (4-5 hours). The volume is reconstructed from tomographic projections

acquired in CBCT using the “back projection” principle, well-known as the Feldkamp Davis Kress (FDK) algorithm [2]. The acquisition leads to noise in the volume due to electronic round-off errors, reduced photon-count, scattering of x-rays, extinction of rays around high-absorbing material, beam hardening as the rays pass through the sample, ring artefacts because of detector pixel malfunction and so on [3, 4]. The analytical reconstruction technique leads to artefacts such as the exponential edge gradient effect where the edges are at high intensity due to the assumption of finite focal spot of the source and aliasing error due to violation of Nyquist sampling. The drift of the sample from the imaging plane, further degrades the image. The quality of the volumes can be improved multifold by fine-tuning the reconstruction algorithms to suit the digital rock domain. Unfortunately, commercial scanners don't provide access to the algorithm for studying the impact of these parameters on the rock samples. To circumvent these issues, we have modified the FDK code available in open access. The code has been incorporated with correction of the angle drift in the sample, which is recorded by the goniometer in the scanner. Positioning of the sample out-of-line of acquisition is inevitable due to its shape and size [5]. The code was also modified to take the center-shift into consideration while executing the reconstruction. This leads to the requirement of a tool to automate the calculation of center-shift, eliminating human decision as to the best value, and is the subject of our future work. The FDK code run time was reduced from 10 minutes to a few seconds by parallelizing the code on GPU and changing the programming language to C. This high-speed code was used to reconstruct the volumes at resolutions higher than the acquired resolution, which is enabled only by this scanner independent FDK algorithm.

- Corresponding author - Dr Jaya Prakash, Department of Instrumentation and Applied Physics, Indian Institute of Science, Bengaluru, Karnataka, India.

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**Poster + / 731**

## Control of chemically-driven convective dissolution by differential diffusion effects

**Author:** Mamta Jotkar<sup>1</sup>

**Co-authors:** Laurence Rongy<sup>2</sup> ; Anne De Wit<sup>3</sup>

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We numerically study the effect of differential diffusion in chemically-driven convective dissolution that can occur upon the reaction of a dissolving species A in a host phase when the chemical reaction destabilises an otherwise stable density stratification. For example, an  $A+B \rightarrow C$  reaction is known to trigger such convection when, upon dissolution into the host solution, A reacts with B present in the solution to produce C if the difference between C and B in the contribution to the solution density is above a critical threshold. We show that differential diffusivities impact the convective dynamics substantially giving rise to additional convective effects below the reaction front, where C is generated. More specifically, we show that below the reaction front either double-diffusive or diffusive-layer convection can arise, modifying the local Rayleigh-Taylor instability. When B diffuses faster than C, a double-diffusive instability can develop below the reaction front, accelerating the convective dynamics and conversely, when B diffuses slower than C, diffusive-layer convection modes stabilize the dynamics compared to the equal diffusivity case. Our results are relevant for various geological applications or engineering set-ups that involve non-reactive stable density stratifications where transport can be enhanced by reaction-induced convection.

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MS19 / 39

## Controlling Gas Diffusion Layer Wettability via Additive Manufacturing and Simulation

**Authors:** Sadeq Saleh<sup>1</sup> ; Sadaf Sobhani<sup>2</sup>

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Chemical exchange and energy storage devices utilize gas diffusion layers (GDLs) to facilitate the transport of gaseous reactants and liquid electrolytes to a catalyst site. The goal of the current work is to study the liquid-gas interface dynamics that result in flooding in GDLs in the context of electrochemical CO<sub>2</sub> reduction (CO<sub>2</sub>R). In CO<sub>2</sub>R reactors, flooding of the porous layer imposes a great challenge in expanding this technology to industrial applications. In fact, flooding of the GDL can happen within several hours of operation, leading to a reduction in selectivity toward CO<sub>2</sub>R reaction products. Generally, flooding is inhibited by hydrophobic coating applied to internal surfaces of the GDL, such as polytetrafluoroethylene (PTFE). However, recent innovations in additive manufacturing and catalyst design have enabled high-performance reactors with unprecedented rates of product conversion. Wettability and the potential for flooding increases as lower surface tension CO<sub>2</sub>R reaction products (e.g., formic acid, methanol, ethanol, and 1-propanol) are introduced in high concentrations into the flowing liquid streams, thus challenging existing GDLs. If the GDL becomes flooded and pores start to fill up with liquid, gaseous CO<sub>2</sub> is blocked from reaching the active site catalyst surface. It is hypothesized that the liquid electrolyte flooding the GDL under high-conversion reactor operation leads to suboptimal performance or even failure of the electrochemical reactor.

We will present a three-dimensional model incorporating the Hoffman expression for dynamic contact angle for CO<sub>2</sub>R products. Next the governing equations will be discretized numerically using the volume of fluid technique in OpenFOAM and executed on a parallel computing platform. The CFD core of this simulation serves as foundation to an optimization algorithm that iterates over the surface texture and morphology of the GDL to study the liquid saturation as a function of capillary pressure. Three morphologies of gyroids, lattice structures, and tubular arrays in combination



with three surface textures of triangular waves, Voronoi embossment, and finned embossments are selected for the purpose of study. The designs are constrained to have equal liquid-gas interface area and contact line length. However, surface texture parameters such as pattern density, chord height, and number of cells per unit volume are unconstrained variables that can be optimized. To update the geometry in each iteration, nTopology software has been used to create a new lattice structure with new sets of input variables. This unique software integration offers a significant advantage over geometry manipulation in OpenFOAM and could be applied to many similar problems involving complex geometry CFD calculations.

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Corral, D., Feaster, J., Sobhani, S. et al. "Advanced Manufacturing for Electrochemical CO<sub>2</sub> Reduction to Multi-Carbon Products." Under Review. **Acceptance of Terms and Conditions:**

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**Poster + / 240**

## Controlling viscous fingering in hierarchal porous media

**Authors:** Harris Rabbani<sup>1</sup> ; Jassem Abbasi<sup>2</sup> ; Ran Holtzman<sup>3</sup> ; Thomas Daniel Seers<sup>1</sup>

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Viscous fingering commonly takes place when a low viscosity fluid displaces a higher viscosity fluid. Although the fundamental principles governing the interfacial pattern in Hele-Shaw cell are well understood, their manifestation in porous media remains elusive. Here, we study viscous fingering in hierarchal porous media (HPM) consisting of a spatially-organized bimodal pore size distribution, namely patches of small and large pores. We use direct numerical simulations and microfluidic experiments to show that viscous fingering, typically highly random, develops into structured interfacial patterns in HPM, in contrast to its random nature in random media. We show that this invasion selectivity highly depends on the flow rate and the pore size contrast. Our results demonstrate that HPM provides a mean to control the morphology of displacement patterns, paving the way towards improved designs of chromatographic columns, membranes, microfluidic devices, and other applications where controlling interface morphology of the displacement pattern in porous materials is desirable.

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## Converging gravity currents of power-law fluids in the subsurface

**Authors:** Sandro Longo<sup>1</sup> ; Luca Chiapponi<sup>1</sup> ; Diana Petrolo<sup>1</sup> ; Alessandro Lenci<sup>2</sup> ; Vittorio Di Federico<sup>3</sup>

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Gravity currents are primarily horizontal flows driven by a density contrast between the current and the ambient fluid. Viscous gravity currents propagate under a viscous-buoyancy balance, inertial forces being negligible except at the very beginning of motion. Non-Newtonian currents arise in several environmental and industrial applications when the fluid has a nonlinear stress-strain relationship. The power-law rheology is the simplest model that approximates the behaviour of a non-Newtonian fluid, in which the strain rate is scaled non-linearly with applied stress. The possibility to have reliable solutions to adopt as benchmarks for the asymptotic behaviour of numerical solutions, and to extract relevant scalings for the front speed and depth of gravity currents, justifies the extension of the analyses already available in literature for a Newtonian case. We hence study gravity currents of power-law fluids of rheological index  $n$  for a particular category of 1-D transient free-surface flow fields that admit self-similar solutions of the second kind. Two different setups in plane ( $x$ ) and radial ( $r$ ) coordinates are examined: i) converging flow toward the origin in a channel of gap thickness  $b(x) \propto x^k$  and  $k < 1$  and ii) converging flow toward the centre in a cylinder. Under the classical viscous-buoyancy balance, the current propagation is described by a differential problem amenable to a self-similar solution. In both configurations, self-similarity requires a transformation identified as a 1-parameter Lie group for which the parameter identification is part of the solution, i.e. an incomplete self-similarity. The time is mapped as  $t_r = t_c - t$ , where  $t_c$  is the touch down time when the converging current reaches the origin. The transformation group is  $U' = U$ ,  $H' = H$ ,  $x' = cx$ ,  $t_r' = c^{1/\delta} t_r$ , where  $U$  and  $H$  are the cross-section averaged velocity and the current depth, respectively. The unknown element of the parameter  $c$  is the exponent  $\delta$ , which is a function of fluid rheology  $n$  and of channel geometry  $k$  for the first setup; it is a function only of  $n$  for the second setup.

For both configurations a single eigenvalue  $\delta_c$  is computed, showing a modest dependency on  $n$ . The theoretical formulation is validated through experiments conducted during both pre- and post-closure phases and aimed at measuring the front position and the profile of the current. Experimental results are in fairly good agreement with theory and allow quantitative determination of the time interval of validity of the intermediate asymptotics regime, when self-similarity is achieved and when is lost.

Both configurations are relevant in subsurface flow in fractures and macropores, and the Hele-Shaw cell with power-law varying gap, configuration i), is directly representative of a porous medium with horizontally varying permeability and porosity, in accordance with the existing analogies valid for power-law fluids. The general layout is also amenable for extension to Herschel-Bulkley fluids and brings to an autonomous system of three variables admitting a spectrum of eigenvalues; this extension is presently under investigation.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

Ciriello, V., Longo, S., Chiapponi, L. & Di Federico, V. 2016 Porous gravity currents: a survey to determine the joint influence of fluid rheology and variations of medium properties. *Advances in Water Resources* 92, 105-115.

Gratton, J. & Minotti, F. 1990 Self-similar viscous gravity currents: phase-plane formalism. *Journal of Fluid Mechanics* 210, 155-182.

Zheng, Z., Christov, I. C. & Stone, H. A. 2014 Influence of heterogeneity on second-kind self-similar solutions for viscous gravity currents. *Journal of Fluid Mechanics* 747, 218-246. **Acceptance of Terms and Conditions:**

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## Correctors and error estimates for reaction-diffusion processes through thin heterogeneous layers

**Authors:** Markus Gahn<sup>1</sup> ; Willi Jäger<sup>1</sup> ; Maria Neuss-Radu<sup>2</sup>

<sup>1</sup> IWR, University of Heidelberg

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Problems including reactive transport processes through thin layers with a heterogeneous structure play an important role in many applications, especially from biosciences, medical sciences, geosciences, and material sciences. In our contribution, we consider a nonlinear reaction–diffusion equation in a domain consisting of two bulk-domains, which are separated by a thin layer with a periodic heterogeneous structure. The size of the heterogeneities and thickness of the layer are of order  $\epsilon$ , where the parameter  $\epsilon$  is small compared to the length scale of the whole domain. In the limit  $\epsilon \rightarrow 0$ , when the thin layer reduces to an interface  $\Sigma$  separating two bulk domains, a macroscopic model with effective interface conditions across  $\Sigma$  is obtained. Here, the scaling of the microscopic model yields an effective reaction-diffusion equation at the interface  $\Sigma$ .

We investigate the quality of the approximation of the microscopic solution by means of the macroscopic one. In general, we cannot expect strong convergence of the gradients or high-order error estimates with respect to  $\epsilon$ . For such results we have to add additional corrector terms to the macroscopic solution which take into account the oscillations in the thin layer and also the coupling conditions between the bulk-regions and the layer. The construction of the approximations is made in two steps. Firstly, we add to the macroscopic solution in the thin layer a corrector of order  $\epsilon$ , which carries information about the oscillations in the layer. This leads to error estimates of order  $\epsilon^{\frac{1}{2}}$  in the  $H^1$ -norms. To obtain a better estimate, in a second step, we add a corrector term of first order to the macroscopic solutions in the bulk-domains and an additional second order corrector to the macroscopic solution in the layer. In the layer, the correctors are obtained by products of the derivatives of the macroscopic solution and solutions of suitable cell problems on a bounded reference element, whereas in the bulk-domains the correctors include solution of boundary layer problems in infinite stripes. The resulting approximation leads to an error estimate of order  $\epsilon$  in the  $H^1$ -norms. The techniques developed in this contribution for reaction-diffusion problems are a first step towards more challenging applications including e.g. advective transport or mechano-chemical interactions.

Andro Mikelić gave significant contributions to the strategy of stepwise building up correctors to improve the effective approximations, especially of solutions to interface problems at the contact between a porous medium and a free fluid, see e.g., the fundamental paper:

W. Jäger and A. Mikelić: On the boundary conditions at the contact interface between a porous medium and a free fluid, Ann. Scuola Norm. Sup. Pisa Cl. Sci. 23:403-465 (1996).

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Time Block B (14:00-17:00 CET) **References:**

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## Coupled LBM-MHFEM simulator for vapor transport in air over a moist soil layer

**Authors:** Jakub Klinkovský<sup>1</sup> ; Radek Fučík<sup>2</sup>

**Co-authors:** Andrew Trautz<sup>3</sup>; Tissa Illangasekare

<sup>1</sup> *Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague*

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**Corresponding Authors:** klinkjak@fjfi.cvut.cz, atrautz@mines.edu, tissa@mines.edu, radek.fucik@fjfi.cvut.cz

We present an efficient computational approach for simulating component transport within single-phase free flow over a soil. A numerical model based on this approach was validated using controlled experiments in a climate-controlled low-speed wind tunnel. The wind tunnel is interfaced with a soil tank to study problems of heat and mass flux across the land-atmospheric interface. The developed modeling approach is based on a combination of the lattice Boltzmann method (LBM) formulated for weakly compressible fluid flow and the mixed-hybrid finite element method (MHFEM) for solving constituent transport. Both those methods individually, as well as when coupled, are implemented entirely on a GPU accelerator in order to utilize its computational power and avoid the hardware limitations that slow communication between the GPU and CPU over the PCI-E bus. We describe the mathematical details behind the computational method, focusing primarily on the coupling mechanisms. Flow and transport simulation results are validated and compared herein with experimentally obtained velocity and relative humidity data based on measurements made above a soil surface over with water evaporates under steady air flow conditions. Model robustness and flexibility is demonstrated by introducing rectangular bluff-bodies to the flow in several different experimental scenarios.

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## **Coupled Thermal-Hydrological-Mechanical-Chemical Model For Reactive Dissolution and Wormhole Formation in Vugs Carbonate Rocks**

**Authors:** Cunqi Jia<sup>None</sup>; Jun Yao<sup>None</sup>

**Corresponding Authors:** rcogfr\_upc@126.com, b17020093@s.upc.edu.cn

Vugs are very common presence in carbonate rocks. According to vugs interconnection, vuggy pore space can be divided into separate-vugs porosity system and toughing-vugs porosity system. Separate-vugs porosity system is also the target rocks for acidizing, in which the addition of vugs only increases the total porosity but has no significant increase of permeability. But few works have been conducted to study effect of vugs on acidizing process.

In this work, a novel two-scale continuum model coupled thermal-hydrological-mechanical-chemical processes is employed to study acidizing process in two typical core-scale separate-vug porosity systems, vugular carbonate rock and isolated vug carbonate rock. Navier-Stokes-Darcy equation is used to describe fluid flow instead of using different equations in free flow region and porous media region. Continuity equation of fluid phase is modified to consider mass exchange between fluid and solid phases. Based on this model, many numerical cases are conducted to discuss a comprehensive vug parametric study on acidizing process and hydraulic behavior including shape, position, filling degrees, and diameter.

Results indicate that acid injection velocity still has an obvious influence on acidizing process when vug exists. Acid consumption volume of vugular carbonate rock and isolated vug carbonate rock are

less than that of matrix carbonate rock, which is consistent with experimental observations. And typical dissolution patterns including ramified wormhole, wormhole, and conical wormhole can also be observed in vug acidizing process. Compared to dissolution patterns of matrix carbonate rock, the presence of vug induces wormhole to pass through vug. The difference of acid consumption mass is generally not obvious with different acid injection velocities both for vugular carbonate rock and isolated vug carbonate rock. Core porosity and permeability both increase as vug porosity and vug diameter increase. But the increasing of core permeability is limited. It further shows that the presence of vug in separate-vug porosity systems only contributes to more storage space but has little contribution for hydraulic conductivity. As for effect of vug porosity and vug diameter on acidizing process, increasing vug diameter and vug porosity can decrease pore volume to breakthrough both for vugular carbonate rock and isolated vug carbonate rock. While in general acid mass does not change a lot.

Vugs provides main storage space for vuggy reserves. However, modeling of vugs is still a challenge until now, which also limits studying of acidizing process in vugs carbonate reservoirs. In this work, a more fundamental two-scale continuum model is developed to study acid transportation and consumption during vugs carbonate acidizing process, which can avoid employing different equations in free flow and porous media regions and determining additional parameters such as material property in BJS condition.

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## **Coupled Thermal-Hydrological-Mechanical-Chemical Model For Reactive Dissolution and Wormhole Formation in Vugs Carbonate Rocks**

**Authors:** Cunqi Jia<sup>None</sup> ; Jun Yao<sup>None</sup>

**Corresponding Authors:** b17020093@s.upc.edu.cn, rcogfr\_upc@126.com

Vugs are very common presence in carbonate rocks. According to vugs interconnection, vuggy pore space can be divided into separate-vugs porosity system and toughing-vugs porosity system. Separate-vugs porosity system is also the target rocks for acidizing, in which the addition of vugs only increases the total porosity but has no significant increase of permeability. But few works have been conducted to study effect of vugs on acidizing process.

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## **Coupled flow and deformation in heterogeneous fractured media: A multirate mass transfer approach for double-porosity poroelasticity**

**Authors:** Sandro Andrés Martínez<sup>1</sup> ; Marco Dentz<sup>2</sup> ; Luis Cueto-Felgueroso<sup>1</sup>

<sup>1</sup> *Universidad Politécnica de Madrid*

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Anthropogenic and natural fractured aquifers are common examples of dual porosity matrix-fracture systems, where the fracture network provides highly-conductive flow pathways and the low-permeability matrix stores most of the fluid. Fluid production or extraction leads to land subsidence and potentially to induced seismicity. Mechanical deformations have recently been proposed as effective monitoring tools for reservoir characterization, complementing flow data.

Coupled flow and mechanical deformation in fractured media is often modeled using the classical theory of dual-porosity poroelasticity (DPP), based on Barenblatt's hypothesis of pressure equilibrium inside the rock matrix blocks. However, classical DPP cannot be expected to upscale flow and deformation in fractured rocks when non-equilibrium effects are relevant. Equilibrium can be expected to appear if the matrix blocks are small, so that the matrix diffusion time is comparable to the flow time scales along the fractures. In practice, matrix blocks may be large enough so that diffusion time scales are long, and the equilibrium hypothesis breaks down.

We study non-equilibrium effects in coupled flow and deformation in fractured media through a theoretical non-equilibrium, dual-porosity model. We use this theory to obtain the scalings for drainage and displacement to be expected for coupled flow and deformation in highly-heterogeneous, fractured porous media. The theoretical model allows to identify what behavior to expect in fractured aquifers and reservoirs, revealing the limitations of classical DPP formulations.

We compare analytical predictions and scalings with high-fidelity numerical simulations, where we describe the coupled flow and deformation for both the rock matrix and a network of discrete fractures, explicitly represented by lower-dimensional (1D) objects. The results show strong tailing in land subsidence and fluid fluxes that cannot be captured by classical DPP or single porosity effective

medium approaches. Conversely, theoretical predictions from the multirate DPP model and the high-fidelity numerical simulations agree, even for highly heterogeneous matrix-fracture systems.

### Acknowledgements

Sandro Andrés gratefully acknowledges funding from the Spanish Ministry of Science, Innovation and Universities (Ministerio de Ciencia, Innovación y Universidades, Programa de Formación de Profesorado Universitario FPU)

### Time Block Preference:

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Andrés, S., Dentz, M., and Cueto-Felgueroso, L. (2021). Multirate mass transfer approach for double-porosity poroelasticity in fractured media. *Water Resources Research*, Under review **Acceptance of Terms and Conditions:**

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## Coupling strategies for free flow with porous media -from single to two phase flow-

**Authors:** Rainer Helmig<sup>1</sup>; Edward (Ned) Coltman<sup>1</sup>; Martin Schneider<sup>1</sup>; Melanie Lipp<sup>None</sup>

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Exchange processes across a porous-medium free-flow interface occur in a wide range of environmental, technical and bio-mechanical systems. In the course of these processes, flow dynamics in the porous domain and in the free-flow domain exhibit strong coupling, often controlled by mechanisms at the common interfaces. Therefore, understanding the underlying processes is decisive. An example of such an environmental problem is soil-water evaporation. The challenge is how we can include scale-dependent, interface-driven processes into mathematical and numerical models for systems of coupled free flow and porous-medium flow.

Based on the excellent work of Andro Mikelic and his co-workers we will discuss the influence of different interfaces for modelling of the coupled systems. In this study, the existing coupling concept is first extended to turbulent free-flow conditions. This includes the interface conditions between a Reynolds-averaged Navier–Stokes free flow using k-omega SST model and a Darcy porous-medium flow. A sensitivity analysis of the evaporation rate and porous-medium quantities on different model setups, boundary conditions, Beavers–Joseph coefficients will be performed. Results demonstrate how turbulence affects the evaporation rate.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

M. Schneider, K. Weishaupt, D. Gläser, W. M. Boon, and R. Helmig. Coupling staggered-grid andmpfa finite volume methods for free flow/porous-medium flow problems.*J. Comput. Phys.*, 401, 2019.  
E. Coltman, M. Lipp, A. Vescovini, and R. Helmig. Obstacles, interfacial forms, and turbulence: Anumerical analysis of soil–water evaporation across different interfaces.*Transport in Porous Media*,134(2):275–301, 2020. **Acceptance of Terms and Conditions:**

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## Data assimilation for reducing uncertainty of subsurface flow modeling using meshless method

**Authors:** Shang-Ying Chen<sup>1</sup> ; Kuo-Chin Hsu<sup>1</sup>

<sup>1</sup> *National Cheng Kung University, Taiwan*

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Since the parametric and predictive uncertainty are inherently inevitable in subsurface flow modeling, various data assimilation methods have been increasingly implemented to constrain the numerical models over the past decade. For example, the Bayes-based ensemble Kalman Filter (EnKF) has been efficaciously applied to updating model pressure state together with hydraulic conductivity by observed pressure data for groundwater modeling, employing uncertainty quantification information based on Monte Carlo or moment equation (ME) method. However, as integrating newly-collected observation data, modelers usually should remesh or refine their original grids to deal with the irregular locations of observation wells. Therefore, the practicality of EnKF may be hindered from tackling a real-world problem due to the lack of numerical method's flexibility. The present study filled the technical gap by utilizing the meshless Generalized Finite Difference (mGFD), which enabled modelers to honor irregular positions by spatially and temporally arbitrary placing computational nodes. The capability of coupled ME-mGFD-EnKF was experimented using scenarios of a two-dimensional transient hypothetical field with pumping tests. The measured conductivity (lnK) data were conditioned via simple kriging to obtain initial inputs, i.e., mean and covariance of lnK; and the mean and covariance of head were calculated by ME-mGFD; then the observed head data were integrated by EnKF to update the so-called augmented state vector, including the mean and covariance of both lnK and head field at each time step. The results show that the parametric and predictive uncertainty can be reduced by using EnKF. Moreover, the results show that present coupled ME-mGFD-EnKF is flexible and promising to accomplish the goal of building a real-time updating subsurface flow modeling for real-world applications.

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## Data driven analysis of evapotranspiration estimated by the water balance and eddy covariance methods

**Author:** Tanja Denager<sup>1</sup>

**Co-authors:** Majken Looms Zibar<sup>1</sup> ; Torben Sonnenborg<sup>2</sup> ; Karsten H. Jensen

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**Corresponding Authors:** tad@ign.ku.dk, khj@ign.ku.dk, mcl@ign.ku.dk, tso@geus.dk

We present the results of a data driven analysis of energy and water balances from one of the field observatories within the Danish Hydrological Observatory HOBE. From this field observatory long time series have been collected of precipitation (several different type of rain gauges), radiation (four component sensors), latent and sensible heat (flux tower measurements using eddy covariance), soil heat flux (heat flux plates), soil moisture (capacity, time domain reflectometry and cosmic ray sensors) and recharge (underground lysimeters). Ideally, both energy and water balance closure should



be obtained when based on the individual measurements. However, it is a well-known problem that a biased imbalance is commonly present between the in- and outgoing energy fluxes when based on the eddy covariance method and evapotranspiration (ET) may therefore be consistently underestimated. ET enters in the energy balance as latent heat flux and in the water balance as water flux and it is therefore possible to cross-check this component. We demonstrate that based on six years of observations ET estimated as a residual term in the water balance equation and ET estimated from the eddy covariance measurements compare well. Thus, we infer that the energy imbalance commonly present when based on the eddy covariance method can likely be attributed to errors in the measurements of the other energy fluxes

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## Data-Driven Finite Element Method, Energy Conservation approach for temperature, water isotope ( $\delta D$ , $\delta^{18}O$ ), and $[SiO_2]_{sat}$ . conc. distributions of the Culex Basin terrestrial hydrothermal system- Yellowstone, WY.

**Author:** Anthony P. Sorensen II<sup>1</sup>

**Co-authors:** Peter B. Larson<sup>2</sup>; Sergey Lapin<sup>3</sup>; Jarred L. Zimmerman<sup>2</sup>

<sup>1</sup> Washington State University-School of the Environment

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The thermal energy distribution of the Yellowstone terrestrial hydrothermal system is driven by a mantle-derived magmatic plume which has both Iron-Magnesium rich and Aluminum-Silicate rich phases and supplies thermal energy to the surface (Crough, 1978). The Yellowstone hydrothermal system is in steady-state within neighborhood of geologic time ( $10^3$  s Ka) and steady-state diffusive nature predominates as the hydrothermal system marches closer towards eruption (Faust, C.R. and Mercer, J.W., 1977). The Yellowstone Plateau Volcanic Field (YPVF) with area on the order of  $90,000 km^2$  is the location of numerous active thermal areas. Since the domains observed during field reconnaissance (2019 and 2020) were relatively small ( \approx  $1.6 km^2$ ) compared to the overall area impacted by thermal energy within the global system (i.e.  $90,000 km^2$ ), care was taken to ensure energy minimization  $1/2 || \nabla(u) ||^2 \approx 0$  within the spatial domain was satisfied during numerical model's implementation of the coupled set of nonlinear hydrodynamic governing equations (i.e. advection-diffusion-reaction) for the observed domain (i.e. Cule Basin). The FEniCS-Dolfin-PETSc numerical libraries were used in the implementation of numerical simulations of spatial distributions for heat, water isotopes (i.e.  $\delta D$ ,  $\delta^{18}O$ ), and saturation silica ( $SiO_2$ ) concentration estimations of the fluid-rock interface observed from Culex Basin hydrothermal features. Energy distributions, thermal and chemical gradient ( $\nabla(u)$ )/numerical flux ( $-K \nabla(u)$ ) fields estimated within the observed fluid-rock interface domain ( $\Omega_{CB}$ ) are the result of the local buoyancy forces (Smith and Chapman, 1983).

If the locally observed hydrothermal systems at Yellowstone interact as energy conservative space time balances, that minimize the distribution of spatial potential energy in the observed phases, then this could be numerical evidence that the global Yellowstone hydrothermal system is in steady-state diffusive energy flux. This would imply that the fluid-rock interface of a terrestrial hydrothermal

system is driven by buoyancy forces which determine fluid velocity fields and thus the elliptic plane of thermal energy distribution decoupled from the physical ground surface (Smith and Chapman, 1983). The finite element numerical results of the nonlinear Lagrange-Galerkin diffusive model for variables measured during field reconnaissance will be discussed for temperature based estimations, and measured spatial distributions and associated flux fields (Sorey et al., 1978).

On terrestrial hydrothermal systems found on Earth, this approach could reduce the amount of exploration drilling needed during geothermal development. Less drilling during said geothermal development could reduce the cost (\$\$) *on the order of hundreds of thousands of dollars. Additionally less drilling could reduce the cost of the Galerkin methods presented, terrestrial hydrothermal system models could be used to compare the data collected from*

### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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California (No. USGS-PP-1044-A). Geological Survey, Sacramento, CA (USA). **Acceptance of Terms**

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### Invited & Keynote Speakers / 809

## Data-based prediction of transport in heterogeneous porous media

**Author:** Masa Prodanovic<sup>1</sup>

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The current barrier to scientific progress in many science and engineering fields is not acquiring data, but efficiently using it for characterization, simulation of transport processes and integration across spatial and temporal scales. In digital rock petrophysics, specifically, advances in high-resolution imaging techniques in the past 30 years have provided a wealth of 2D and 3D datasets that reveal the microstructure of and transport phenomena in rocks and soil on scales ranging from nanometers to centimeters. Many of those are curated in Digital Rocks Portal, <https://www.digitalrockportal.org/>.

I present a novel multiscale deep learning model that is able to learn from large number of images of porous media (harvested from Digital Rocks Portal) and data resulting from related high-performance computing. The main novelty is ability to perform accurate inference of large computational domains exhibiting heterogeneity thanks to its efficient architecture of linked neural networks. The model opens up the possibility of solving domain sizes that would not be feasible using traditional direct simulation tools on a desktop computer, as well as integrating multiple imaging scales available. The method is validated with a laminar fluid flow case using vuggy and fractured porous samples. The focus of the present work is validating single phase flow application, but the methodology should be applicable to many other transport problems where geometry has the first

order influence. I finally discuss integration of both geometry and wettability information in predicting two phase flow in fractures.

The presented work is collaboration with J. E. Santos, Y. Yin, , H. Jo, W. Pan, M. Pyrcz, N. Lubbers, H. Viswanathan, E. Gultinan and Q. Kang.

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## **Deep Learning-based sensitivity analysis for subsurface flow and transport**

**Author:** Jonghyun Lee<sup>1</sup>

**Co-authors:** Vincent Liu<sup>2</sup> ; Hongkyu Yoon<sup>2</sup>

<sup>1</sup> *University of Hawaii at Manoa*

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Accurate modeling and prediction of flow and reactive transport in fractured and porous media under uncertainty requires characterization of unknown model parameters such as permeability, hydrodynamic dispersion coefficient, and/or reaction kinetics, with their estimation uncertainty. Sensitivity analysis of such parameters plays an important role before or during the uncertainty analysis by checking whether one has enough information to identify a parameter given uncertainty of other parameters and hence reducing the number of parameters to be estimated. In this work, we propose local and global sensitivity analysis methods using a deep learning-based approach. With advancements in computational power and open-source programming packages, deep learning can offer computationally efficient reduced-order models to the flow and reactive transport problem. With automatic differentiation, trained deep learning models can produce local sensitivity, i.e., the gradient of the forward model output with respect to the observation, in the order of seconds and the expensive computation of global sensitivity such as Moris and Sobol indices is computationally feasible. In specific, we use physics-informed neural network approaches to offer local and global sensitivity analysis. Since such analysis tells which parameters are informative for optimal experimental design with data-worth analysis, decision makers can allocate limited budgets optimally to collect field observations for future site characterization.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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**MS15 / 83**

## Deep learning enhancement of micro-CT images for large-scale flow simulation

**Author:** Samuel Jackson<sup>1</sup>

**Co-authors:** Yufu Niu<sup>2</sup>; Sojwal Manoorkar; Peyman Mostaghimi; Ryan Armstrong

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There are inherent resolution and field-of-view trade-offs in X-Ray micro-computed tomography imaging, which limit the characterization, analysis and model development of porous systems with multi-scale heterogeneities. In this work, we overcome these tradeoffs by utilising a deep convolution neural network to create enhanced, high-resolution data over large spatial scales from low-resolution data.

We use paired high-resolution (2 micrometres) and low-resolution (6 micrometres) images from two structurally-different Bentheimer rock samples to train an Enhanced Deep Super Resolution (EDSR) convolutional neural network. The generated high-resolution images are validated against the true high-resolution images through textual analysis, segmentation behaviour and pore-network model (PNM) multiphase flow simulations. The final trained EDSR network is then used to generate high-resolution digital rock cores of the whole samples with dimensions of 1.2cm × 1.2cm × 6-7cm. The 3D digital rock cores are populated with continuum properties predicted from subvolume PNMs, and used to simulate a range of experimental multiphase flow experiments. We present a consistent workflow to analyse multi-scale heterogeneous systems that are otherwise intractable using conventional methods.

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## Deep learning for digital rock image segmentation in pore structure characterization

**Authors:** Jiuyu Zhao<sup>1</sup>; Jianchao Cai<sup>2</sup>

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Accuracy of rock image segmentation is the base of digital rock, and decides the credibility of subsequent physical calculation. However, it spends much time to acquire perfect segmentation result. Benefitting from the advances in hardware and algorithms, deep learning has been widely used in image process for it doesn't need the complex image preprocessing comparing with conventional segmentation method. In this work, Segnet, a deep convolutional encoder-decoder architecture for image segmentation, was used to classify pore, matrix or fluid phase in CT images. Two datasets are used to demonstrate the capability of Segnet: the shale images conduct to distinguish two phases (pore and matrix), and the Doddington sandstone data is used to divide into three phases (pore, matrix and fluid phase). Each dataset is composed by 3000 images with 256×256 voxels respectively,

80% of them was used for training, 10% for testing and 10% for validation. The accuracy of segmentation of each phase on validation dataset is great than 90%, the pore structure extracted from segmental images, such as porosity and fractal dimension, have little difference comparing with experimental result. The results demonstrate that the deep learning is applicable and greatly potential for segmentation in digital rock.

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## Deep-learning-based Image Segmentation Techniques for Porous Media Property Estimation

**Authors:** Yuhan Hsi<sup>1</sup> ; Fangya Niu<sup>1</sup> ; Prakash Purswani<sup>1</sup> ; Xiaolei Huang<sup>1</sup> ; Zuleima Karpyn<sup>1</sup> ; Parisa Shokouhi<sup>1</sup><sup>1</sup> *The Pennsylvania State University***Corresponding Authors:** pxs990@psu.edu, fun31@psu.edu, pxp5185@psu.edu, zkarpy@psu.edu, suh972@psu.edu, ybh5084@psu.edu

Recent advances in image data science, data storage and high-performance computing have enabled the application of machine learning and data-driven approaches to a wide range of disciplines. Image data analysis in the geosciences and phase identification from core analysis have allowed significant developments in the characterization of structural, compositional, storage and transport properties. We present a deep-learning based approach for automated segmentation of solid, brine and CO<sub>2</sub> phases in a porous media sample imaged by X-ray microCT. The porous sample consisted of a sintered glass frit, 12mm diameter, 25.36mm long, 30% porosity and 630mD permeability. The sample was subject to multiple injection cycles of brine and CO<sub>2</sub> at supercritical conditions. MicroCT images were acquired at two quality levels, high and low (fast scan), both at a voxel resolution of 15µm. In order to train a machine learning model to perform automated segmentation on both high-quality and low-quality images, ground truth segmentation examples are needed as training data. We obtain the training data by utilizing an interactive segmentation method based on a Random Forest classifier, which takes user-input examples of voxels from different phases and generates a full-segmentation map that labels every voxel in an image. The interactive segmentation of high-quality images provides us with ground-truth segmentation maps. Once the ground truth annotations are acquired, we prepare training data, which consist of image and annotation pairs: high-quality image and segmentation annotation, low-quality image and segmentation annotation. High- and low-quality images are different scans from the same experiment, thus correspond to the same ground-truth. To accurately segment the images, we experimented with several supervised and semi-supervised neural networks, including U-Net, SegNet, and DenseUNet, which are deep learning models that can be trained to take a raw image as input and generate the segmentation map as output. We report our findings that compare several state-of-the-art segmentation models using cross validation and demonstrate that a deep learning model trained for automatically segmenting microCT images can achieve high accuracy and is generalizable to segmenting images of different quality, resolution and from different porous media samples. Based on the segmentation results, we also calculate sample properties such as pore topology, porosity and saturation, and compare such estimates from high-quality vs. low-quality images. In our future work, we will investigate the training of machine learning models that can reliably identify and segmentation different phases in rock samples that have different mineral composition and structural features. We will also study machine-learning-based super resolution algorithms that can generate super high-resolution images from low-resolution images.

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MS15 / 391

## Deep-learning-based surrogate model for brine extraction well placement for geological carbon storage

**Authors:** Hyunjee Yoon<sup>None</sup> ; Yeongju Kim<sup>None</sup> ; Hoonyoung Jeong<sup>1</sup> ; Alexander Sun<sup>2</sup> ; Bo Ren<sup>3</sup>

<sup>1</sup> *Seoul National University*

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In a geological carbon storage project, management of reservoir pressure buildup is essential for long-term safe carbon storage. A reservoir pressure buildup caused by CO<sub>2</sub> injection may lead to serious safety issues such as induced seismicity, caprock damage, and leakage of brine and CO<sub>2</sub>. Brine extraction is a practical solution to mitigate the reservoir pressure buildup. In heterogeneous reservoirs, the performance of brine extraction is significantly affected by where to place a brine extraction well because the mitigation of pressure buildup and the arrival time of injected CO<sub>2</sub> to the brine extraction well are determined by the hydraulic connectivity map. The optimization of a brine extraction well location is computationally expensive because many reservoir simulation runs are required to seek optimal locations in potential well locations. We propose an efficient surrogate model that computes the optimality of a brine extraction well quickly using the fast marching method and a convolutional neural network. The arrival time map of a pressure pulse that the fast marching method provides rapidly can be used as a good representation of the hydraulic connectivity map for a brine extraction well location. The performance of our surrogate model is demonstrated in a CO<sub>2</sub> injection site in the Pohang basin. The computational cost of optimization of a brine extraction well is significantly saved using our accurate surrogate model compared to a normal optimization process.

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## Deformation-driven solute transport in soft porous media

**Authors:** Matilde Fiori<sup>1</sup> ; Chris MacMinn<sup>1</sup> ; Satyajit Pramanik<sup>2</sup>

<sup>1</sup> *University of Oxford*

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Solute transport plays an important role in many soft porous materials, including the movement of contaminants in soils and the movement of nutrients and waste in living tissues and tissue-engineering scaffolds. These systems are also often exposed to large, periodic loading and deformation, which drives nontrivial fluid motion and changes in pore structure. Here, we study the strong coupling between fluid flow and mechanical stimulation during periodic deformations using a 1D continuum model based on large-deformation poroelasticity. We show that these reversible deformations lead to non-reversible spreading and mixing, even in a homogeneous medium. We analyse the three primary mechanisms of solute transport (advection, molecular diffusion, and mechanical dispersion) and study their separate impacts on the solute distribution. We also identify the key dimensionless parameters that govern deformation-driven transport, and we study their qualitative and quantitative impacts on solute spreading and mixing.

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MS7 / 181

## Density instabilities due to evaporation from porous media

**Authors:** Carina Bringedal<sup>1None</sup> ; Cornelis J. van Duijn<sup>1</sup> ; Gert-Jan J. M. Pieters<sup>2</sup> ; Rainer Helmig<sup>3</sup> ; Theresa Kurz<sup>None</sup>

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We consider a porous medium in a semi-infinite domain, saturated with saline water. The top boundary is subject to evaporation of water but where the solute stays behind, while the bottom boundary has an inflow of water with the background solute concentration. This leads to an accumulation of solute near the top boundary. As the density of the water increases with larger solute concentration, this setup is gravitationally unstable. Hence, convective instabilities in the form of fingers can occur due to the arising density difference. However, these instabilities will only occur if the density difference is large enough to overcome the stabilizing effects from diffusion and viscous forces. In certain cases the solute could precipitate before instabilities manage to develop.

We address this instability problem by applying the well-known Boussinesq approximation and performing a linear stability analysis. Through solving the arising eigenvalue problem, we obtain criteria for when instabilities can develop. For given parameters as evaporation rate, permeability of the medium and initial solute concentrations, we can give criteria for when - or whether - instabilities develop. The criteria coming from the eigenvalue problem is compared with results from numerical simulations.

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MS9 / 604

**Determination of Characteristic Transport Coefficients of Porous Media: A Diffuse Interface approach****Author:** Chahat Aggarwal<sup>1</sup>**Co-authors:** Amin Sadeghi ; Elizabeth Monte <sup>1</sup> ; James Lowman <sup>1</sup> ; Jeff Gostick <sup>1</sup> ; Nasser Mohieddin Abukhdeir <sup>1</sup><sup>1</sup> *University of Waterloo***Corresponding Authors:** ejmonte@uwaterloo.ca, amin.sadeghi@uwaterloo.ca, jlowman@uwaterloo.ca, nmabukhdeir@uwaterloo.ca, jgostick@uwaterloo.ca, c2aggarw@uwaterloo.ca

Fluid mechanics simulations of flow through porous media frequently use the Lattice Boltzmann Method (LBM) due to its compatibility with experimentally determined volumetric images of porous media. However, the use of the LBM does present challenges including accuracy of the fluid/solid interface and complexity of determining Lattice Boltzmann formulations for varying transport models. Traditional finite element-based methods require conformal meshes of porous domains that are able to accurately capture fluid/solid interfaces, but at the cost of significant computational complexity and user-interaction in order to create the mesh.

To address these challenges, this work presents the application of a diffuse-interface finite element method that approximates a phase-field from 3D tomography voxel images without user interaction and enables the use of a simple structured grid/mesh for traditional finite element-based fluid mechanics methods. The presented diffuse interface method is automated and non-iterative, enabling the direct calculation of three characteristic coefficients from an input tomogram: tortuosity, permeability, and inertial constant, optionally for each direction by simulating Fickian diffusion and single component incompressible Navier Stokes equation from low to high range of Reynolds numbers. The method is compared to traditional FEM implementation using conformal meshes with respect to the agreement with experimental determination of the characteristic coefficients, numerical accuracy, and computational requirements (time and memory). It was found that for comparable computational complexity, the diffuse interface method provides more accurate results than that of the conformal mesh approach. The developed method provides an automated and computationally feasible approach for computing effective transport properties from tomograms.

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MS6-A / 394

**Developed emulsification in porous media flow****Authors:** Ahmad Kharrat<sup>None</sup> ; Bianca Brandstätter<sup>1</sup> ; Rene Ritter<sup>1</sup> ; Mostafa Borji<sup>2</sup> ; Pit Arnold<sup>None</sup> ; Gerhard Popovski<sup>1</sup> ; Oskar Paris<sup>3</sup> ; Holger Ott<sup>1</sup><sup>1</sup> *Montanuniversität Leoben*<sup>2</sup> *Montanuniversität Leoben*<sup>3</sup> *Montanuniversität leoben*



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With the use of surfactants, the interfacial tension between oil and water can be lowered to a degree that solubilisation of oil by injection water leads to a near-miscible displacement. However, the resulting emulsification depends on the mechanisms of how the two phases contact each other and ultimately on the mixing, respectively, flow regime. While in classical test tube experiments, mixing might be turbulent, under laminar flow conditions in a porous medium, miscibility may slowly develop over time, depending on dispersive mechanisms facilitating the contact between the phases. The present study investigates the developed miscibility during surfactant flooding. We perform microfluidic experiments with generic fluids and surfactant and salt concentrations, as reported in earlier studies. We observe emulsification and oil displacement in-situ and under flow conditions by optical and fluorescence microscopy. Additionally, emulsion phases were characterized by ex-situ auxiliary measurements to determine the principal phase behaviour, interfacial tension and droplet sizes.

During displacement, a sequence of displacement mechanisms and emulsion phases were observed, with the exact mechanism depending on the water salinity as a tuning parameter. At the leading front, a slight capillary instability is observed, microscopically bypassing oil and hence forming residual oil clusters. This effect is minimized at optimum salinity, leading to the best displacement efficiency. The front is followed by a phase that may be described as foam-like before a connected emulsion phase appears solubilizing ultimately remaining oil behind the displacement front. This foam-like structure facilitates a patchy, non-uniform emulsion phase with respect to phase composition (oil in water concentration). On the way to the connected emulsion phase, events are observed, that may be described as the coalescence of water droplets or alternatively, as a collapsing foam phase. The complex spatial and temporal phase distributions may cause complex flow properties at the displacement front with respect to fluid-phase mobility, which requires additional research. In the presentation, we discuss a first characterization attempt.

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MS18 / 479

## Development of a new complex fluid for DNAPL recovery and nZVI delivery

**Authors:** Sagyn Omirbekov<sup>1</sup>; Stéfan Colombano<sup>2</sup>; Amir Alamooti<sup>3</sup>; Azita Ahmadi-Senichault<sup>4</sup>; Hossein Davarzani<sup>2</sup>

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Soil contamination is one of the challenging problems that present risks for both the environment and the general population. Manufactured products made by chemical plants commonly contaminate aquifers and soils with miscible and immiscible organic liquids. In particular, in-situ remediation of soil contaminated with Dense Non-Aqueous Phase Liquids (DNAPLs) is of great interest. They represent one of the major pollutants found in France and other industrial countries (Colombano et al. 2020). Since DNAPL is denser than water, it commonly migrates vertically downward through the saturated zone until its displacement is hindered by low permeable formations where

it starts to migrate laterally. These mechanisms will form DNAPL pools over the low permeability zones (Huling, 1991).

The displacement of DNAPL with low-density and less-viscous solutions is less efficient due to a complex interplay among viscous, gravity, capillary, and buoyancy forces. Therefore, it is nearly impossible to recover all DNAPL and avoid the back-diffusion effect (Seyedabbasi et al., 2012). Moreover, the classical pump and treat method is inefficient due to the low recovery yields below 60% (Colombano et al. 2020). Therefore, complex fluids, including foam and polymer solutions, were recently used (Maire et al., 2019; Omirbekov et al., 2020) for soil remediation. However, mobilization of DNAPL with less-dense fluid is doubtful because of higher buoyancy forces within the contaminated site. Consequently, the effect of denser polymer solutions on DNAPL mobilization is unknown. In this work, we investigate barite use to densify polymer solutions and apply this solution to transport nano-scale zerovalent iron (nZVI) to remediate soil contaminated with pure heavy chlorinated organic compounds.

To embody the concept, several environmentally-friendly polymers (guar gum, xanthan gum, and carboxymethyl cellulose) were experimentally studied to find their stability with barite (97% of BaSO<sub>4</sub>) and nZVI. The interfacial tension and rheological behavior of the solutions were examined. Furthermore, we carried out 1D porous column (filled with 0.5 mm glass beads) experiments to investigate the DNAPL displacement in porous media with the polymer, barite-polymer, and nZVI-barite-polymer solutions.

According to the decantation tests, the stability of nZVI and barite densified polymer solutions are ranked as the following: carboxymethyl cellulose > guar gum > xanthan gum. The column test shows that the polymer solution based on barite and carboxymethyl cellulose with the same density of DNAPL has the best recovery efficiency (up to 95%). Moreover, this solution allows delivering the nZVI while displacing the chlorinated compounds to reduce and degrade the DNAPL residual saturation.

Our results demonstrate the effectiveness of the new slurries for soils contaminated with DNAPL. Therefore, the newly developed solution can be directly injected into the DNAPL contaminated zones, improving the remediation rate and decreasing the economic cost. We anticipate that our research will constitute a starting point for developing new environmental fluids to remediate soils contaminated by DNAPL.

#### **Time Block Preference:**

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Colombano, S., Davarzani, H., van Hullebusch, E.D., Ignatiadis, I., Huguenot, D., Omirbekov, S., Guyonnet, D.: Free Product Recovery of Non-aqueous Phase Liquids in Contaminated Sites: Theory and Case Studies. In: van Hullebusch, E.D., Huguenot, D., Pechaud, Y., Simonnot, M.-O., and Colombano, S. (eds.) *Environmental Soil Remediation and Rehabilitation: Existing and Innovative Solutions*. pp. 61–148. Springer International Publishing, Cham (2020)

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Seyedabbasi, M.A., Newell, C.J., Adamson, D.T., Sale, T.C.: Relative contribution of DNAPL dissolution and matrix diffusion to the long-term persistence of chlorinated solvent source zones. (2012). <https://doi.org/10.1016/j.jconhyd.2012.03.010> **Acceptance of Terms and Conditions:**

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**Development of a simple-to-use and novel correlation to predict apparent viscosity of waxy crude oils mixed with polymeric ad-**

## Abstracts

**Authors:** Mohammad Madani<sup>1</sup> ; Maryam Hasanzadeh<sup>2</sup>

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Although several investigations on the waxy crude oils have been conducted, there are no adequate research studies on the prediction of the apparent viscosity of waxy crude oils mixed with polymeric inhibitors. In this study, multi-gene genetic programming (MGGP) as a powerful intelligent model is used to develop an accurate and efficient mathematical model to relate process input parameters to the output for predicting the apparent viscosity of waxy crude oils doped with polymers. The new proposed mathematical model is evaluated by a large collected data set from the published literature. The total collected datapoints are randomly divided into three subcategories; 70% for training, 20% for testing, and 10% for validation stages. The high accuracy and reliability of the new proposed model to predict the apparent viscosity is confirmed by the calculated statistical parameters. The values of R-squared for training, testing, and validation steps are 0.98819, 0.96491, and 0.98501, respectively. The statistical assessments show the high accuracy and reliability of the developed model. The new proposed mathematical model can be used to predict the apparent viscosity of waxy crude oils doped with polymeric additives with high accuracy without requiring expensive and time-consuming experimental investigations.

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## Development of flow through cell method for in-situ visualization of dissolution processes in solid dosage forms

**Authors:** Niloofar Moazami Goudarzi<sup>1</sup> ; Aseel Samaro<sup>2</sup> ; Chris Vervaeet<sup>2</sup> ; Matthieu Boone<sup>1</sup>

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In the pharmaceutical industry, different methods have been developed to analyze the internal structure of solid dosage forms such as mercury porosimetry, and gas adsorption (1,2). These methods are destructive and unable to study the dynamic property of a sample during dissolution. Hence there is a growing demand for developing non-destructive techniques to visualize and characterize the internal structure of dosage form during the dissolution process. X-ray tomography is one such technique that has been used to monitor structural change during the dissolution process, mostly by halting the process and drying the sample before the imaging (3). However, these processing steps could change the internal structure.

In this work, dynamic X-ray  $\mu$ CT imaging was used to monitor and analyze the dissolution of a 3D printed tablet. A flow-through cell was developed to mimic the in-vivo dissolution process, and enables us to visualize the internal structure of pharmaceutical tablets during the process. To increase the attenuation contrast between water and the tablet, CsCl was used as the contrast agent. Finally, we investigated the correlation between drug release calculated from in-vitro dissolution and the results from 4D- $\mu$ CT.

Conventional dissolution tests were performed to investigate the impact of CsCl brine on the dissolution rate of active pharmaceutical ingredient (API) from the tablets: one using CsCl brine (PH=6.6) as dissolution medium and the other in a phosphate buffer (PH=6.8). The dissolution profiles of tablets in different mediums were compared. The result shows that the effect of CsCl brine on the dissolution profile is negligible.

The Environmental Micro-CT (EMCT) scanner of the Ghent University Centre for X-ray Tomography was used for imaging (4). The tablets were scanned with a temporal resolution of 2 minutes for a full rotation, and a spatial resolution of 20  $\mu\text{m}$ . X-ray  $\mu\text{CT}$  scans were acquired at dry state, at the time that medium filled the flow cell, and several time steps ranging from 0.25 to 7 hours of the dissolution. Immediately after each scan, 5 ml of solution was taken and analyzed by UV spectrophotometer at 222 nm ( $\lambda_{\text{max}}$  MPT in CsCl brine) to measure the concentration of released API. All scans were reconstructed using filtered backprojection as implemented in Octopus Reconstruction. Octopus Analysis was used for the 3D analysis of the reconstructed scans. From segmenting the wetted region, the volume of penetrated water was determined.

The API release shows a linear relation to water penetration to the tablet (which is reflected by an increase in local X-ray attenuation coefficient due to the penetration of the brine into the dosage form), suggesting that the slope of this line can be used to convert the image data to the amount of API released from the tablet. This study demonstrates the potential of X-ray  $\mu\text{CT}$  to examine the internal structures of pharmaceutical tablets during the dissolution process. The advantage of the proposed method is that the dynamic property of dosage form during the dissolution process can be assessed without further sample preparation.

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MS4 / 734

## Diffusion of water in palm leaf materials

**Authors:** Debapriya Pinaki Mohanty<sup>1</sup>; Anirudh Udupa<sup>1</sup>; Mysore Dayananda<sup>2</sup>; Srinivasan Chandrasekar<sup>1</sup>

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Diffusion of water into plant materials is known to degrade their mechanical strength and stiffness, yet simultaneously enhance formability. Hence, the phenomenon is of both fundamental interest, and of importance for manufacture of eco-friendly products, e.g., foodware (plates, bowls). The existing literature on diffusion in plant materials (mainly woods) has focused on diffusion of water vapor (moisture) rather than liquid water. Furthermore, these studies have largely been restricted to estimating the macroscopic diffusion coefficient, using measurements of mass gain, with little

focus on elucidating the micro-mechanisms of diffusion. Given the complex hierarchical structure of plant materials, the diffusion process may be expected to be strongly influenced by microstructural components such as fiber, matrix and porosity. Even a qualitative understanding of the role of microstructure in influencing diffusion of water will be of value for predicting the response of plant materials to water permeation, without extensive macroscopic measurements.

Here, we report on measurements of diffusion coefficient of water in areca palm sheath, a model plant material system, also used in eco-friendly foodware. The measurements account for the effects of material swelling and porosity, unlike prior characterization of this diffusion. Using in situ imaging, we show that the permeation of water through the sheath microstructure occurs heterogeneously, being several times faster in the matrix than in the fibers. Furthermore, using digital image correlation (DIC), we map the variation in the local strain during the diffusion process and show that it is significantly higher in regions of greater water penetration. The diffusion coefficient obtained from conventional mass gain measurements is shown to be consistent with the observations from the imaging experiments. The results highlight the critical need to include microstructure parameters, such as porosity and material swelling, to accurately estimate the diffusion coefficient. Implications of the results for diffusion in hierarchically structured materials, foodware manufacturing, and life of foodware products are discussed.

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## Digital Rock Analysis of Low Resistivity Pay Zones to Refine Saturation

**Authors:** Ivan Deshnenkov<sup>1</sup>; Aqeel Furaish<sup>None</sup>; Hussain Alhilal<sup>None</sup>

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Low resistivity pays (LRPs) are reservoirs from which dry hydrocarbons are produced in the presence of erroneously interpreted water saturations. LRP are often identified within laminated reservoir sequences, shaley lithologies, and formations with multi-modal pore-size characteristics or containing fresh formation waters identified on the basis of well logging, testing and core observations. The following study addresses the characterization of a microporous carbonate LRP formation using digital rock physics (DRP) analysis in various facies identified in 62 core plugs through digital imaging. A comprehensive DRP workflow was utilized to produce 3D digital rock models of rock samples through multi-resolution X-ray tomographic imaging and application of a machine-learning algorithm to characterize the internal fabric of the rock samples based upon the abundance of microporosity. The physical samples were also analyzed using mercury injection capillary pressure (MICP) to allow calibration and validate the 3D digital rock models. Numerical simulation of the electrical current flow through the samples showed the variation of Archie's saturation exponent "n" with water saturation, i.e., the increasing influence of the microporous regions as water saturation is decreased. The meso- and macro-pores were found to produce the moveable hydrocarbons due to their lower capillary pressure; the micro-pores holding immobile formation water. The DRP models were then used to simulate the drainage relative permeability curves to identify the water saturation causing the first water in-flow, and separate immobile and free-fluids. The wireline logs saturation profile was updated with these results.

As shown by digital experiments, conducted on LRP the water-filled micro-pores provide a continuous path for electric current, masking the hydrocarbons and overestimating the water saturation. Saturation calculation could be significantly refined, if LRP wireline petrophysical models are calibrated using DRP data incorporating the modelled Archie's saturation exponent and first water in-flow from relative permeability curves.

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Poster + / 636

## Digital Rock Typing

**Authors:** Omar Al-Farisi<sup>1</sup> ; Mohamed Sassi<sup>2</sup> ; Djamel Ouzzane<sup>3</sup><sup>1</sup> *Khalifa University of Science and Technology*<sup>2</sup> *Khalifa University*<sup>3</sup> *ADNOC***Corresponding Authors:** djouzzane@adnoc.ae, alfarisi@live.ca, mohamed.sassi@ku.ac.ae

Towards the quest for accuracy and efficient characterization of heterogeneous cretaceous carbonate, the path for geology and data scientists is full of challenges. The main challenge for achieving both accuracy and efficiency simultaneously is the ability to have the machine understand the heterogeneity effect on the rock's physical properties. From rock micro-Computed Tomography (uCT) images to rock types, we propose a fully artificial intelligence-based workflow. We enable the machine to identify the pore throat heterogeneity types, determine the rock's physical static properties; porosity, lithology, permeability, and capillary pressure, then finally classify the rock types using the novel Carbonate Morphology Chart, CAMO Chart.

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MS9 / 175

## Digital rock approach for unconsolidated sandpacks using pore network modelling: comparison between experiments and simulations

**Author:** Erika Shiota<sup>1</sup>**Co-authors:** Takashi Akai<sup>1</sup> ; Michiharu Hiyama<sup>1</sup><sup>1</sup> *JOGMEC***Corresponding Authors:** hiyama-michiharu@jogmec.go.jp, akai-takashi@jogmec.go.jp, shiota-erika@jogmec.go.jp

Multiphase flow properties such as the capillary pressure and the relative permeability are a crucial parameter for subsurface evaluation and engineering such as oil & gas development and CCS projects. The measurement of the relative permeability of unconsolidated rocks is extremely difficult due to the collapse of samples and the influence of changes in the internal structure due to particle movement during the test. In addition, there have been few examples of relative permeability measurements using unconsolidated rocks due to the difficulty in handling test and spend a long time.

On the other hand, the research has been conducted to extract pore structure with micro X-ray CT imaging. These images can be used to extract a pore network model (PNM) which can be used to obtain the capillary pressure and relative permeability of rocks [1] [2]. Thus, the purpose of this study is to quantitatively evaluate the capillary pressure and relative permeability of unconsolidated sandstone by applying the PNM. In this contribution, we show the results of the validation of the method to quantitatively evaluate the absolute permeability and the capillary pressure of unconsolidated sandstone by applying the PNM to unconsolidated rocks.

To evaluate the validity of the method, sandpacks were prepared using single-grained sands to simulate a unconsolidated sandstone, and CT images of the sandpacks were acquired. And to evaluate the validity of the PNM, the pore structure was extracted from the CT images and the PNM was developed. This presentation will show the comparison of the absolute permeability and capillary pressure between experimental measurements and simulations. First, the absolute permeability obtained with the PNM was fairly consistent with that measured on the different packs composed of the same sand grains. Furthermore, it gave a good agreement with the permeability obtained by direct numerical simulation performed on the pore structure extracted from the same CT images. Next, we compared the capillary pressure and relative permeability obtained by the PNM with the experimental values. When a water-wet system was assumed, the simulated values showed a good agreement with the experimental values.

From these results, it is concluded that the fluid parameters of unconsolidated sandstone can be obtained simply by constructing the PNM.

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## Direct Pore-scale Simulation of Thermal-Hydraulic-Mechanical Coupling Effect on the Process of Waterflooding with FVM Method

**Authors:** Shaobin Cai<sup>None</sup> ; Yongfei Yang<sup>None</sup> ; Jun Yao<sup>None</sup>

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Research on the thermal-hydraulic-mechanical (THM) coupling effect in porous media from the perspective of pore-scale is of great significance for the study of enhanced oil recovery, nuclear storage and geological sequestration of CO<sub>2</sub>. The flow of multiphase fluid in porous media is affected by the thermal-hydraulic-mechanical coupling effect, and the interaction of multiple fields brings about the complex interface phenomenon between fluid-fluid and fluid-solid and the change of fluid properties. We proposed a Darcy-Brinkman-Biot (DBB) combined with a Conjugate Heat Transfer (CHT) method to model water-oil two-phase flow under the THM effect in porous media. The DBB method was used to simulate the HM process, by characterizing the fluid-structure interaction of two-phase flow in porous media considering matrix deformation. For the free flow in the pore space, the N-S equation was solved, while for the fluid flow in the matrix, the Darcy equation was solved. At the same time, the CHT method was adopted to consider the heat transfer between the matrix and the pore space during the flow process. Good agreements were achieved by comparing our simulation results with the theoretical results through the simulation of the simple classical model, thus verifying our model. Finally, we established two kinds of models, one is an ideal two-dimensional porous media model, and the other one is a slice model extracted from a three-dimensional digital

core model based on micron-CT scanned and reconstructed image, to study the effects of different injection PV (pore volume) numbers on the distribution of two-phase fluid, pore structure, and temperature.

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## Direct Visualization of Induced Asphaltene Removal in Carbonate Rock Using Confocal Imaging

**Authors:** Mahmood Amani<sup>None</sup> ; Arnel Carvero<sup>None</sup> ; Harris Rabbani<sup>1</sup>

<sup>1</sup> *Texas A&M University at Qatar*

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Asphaltenes deposition can have a detrimental impact on hydrocarbon recovery efficiency. Therefore, it is imperative to study the fundamental mechanisms controlling the asphaltene flocculation and deposition in reservoirs. The primary objective of this study is to visualize the deposition of asphaltene and their subsequent removal by ultrasonication in Indiana Limestone using state-of-the-art confocal microscopy. To do so, we performed a comprehensive series of experiments by flooding Indiana Limestone core samples with crude oil and later passing ultrasonic waves through the flooded sample. At each stage of experiment series of images were captured by confocal microscopy depicting asphaltene deposition and its post-sonication distribution. The comparison of confocal scans reveals that the ultrasonic irradiation is highly efficient in removing asphaltene from the low permeability core samples.

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Direct Visualization of Ultrasonication Induced Asphaltene Removal in Carbonate Rock Using Confocal Imaging (2020). Mahmood Amani, Harris Sajjad Rabbani, Arnel Carvero, Dilyara Iskakova, Rommel Yrac. Petroleum and Chemical Industry International. ISSN: 2639-7536 **Acceptance of Terms and Conditions:**

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MS25 / 307

## Dispersive effects in buoyancy-driven flow including plume-fed gravity currents

**Author:** Saeed Sheikhi<sup>1</sup>

**Co-author:** Morris Flynn<sup>2</sup>

<sup>1</sup> *PhD student, University of Alberta*

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Buoyancy-driven flow in porous media is bookended by two canonical scenarios: a vertically-descending plume and horizontally-propagating gravity current. Whereas the former is dominated by entrainment, the latter often includes significant dispersion. For example, when a gravity current propagates down-dip along a permeability jump (sloping or horizontal), the leading edge may fractionate into bulk and dispersed interfaces. Sahu and Neufeld (J. Fluid Mech., Vol. 886 ,2020) studied dispersive effects and gravity current flow both theoretically and experimentally. They considered dispersive effects only in the transverse direction and not in the longitudinal direction. Aiming to expand upon their pioneering study, we wish to investigate dispersive effects both parallel and perpendicular to the principle direction of flow. To this end, we developed a COMSOL model to study miscible buoyancy-driven flows in porous media in which different categories of flow arise. These categories include plume flow, gravity current flow and drainage from an upper layer of high permeability to a lower layer of low permeability. Our model is validated by comparing the numerical results with existing experimental data. We exploit this model to study the effects of dispersive entrainment in directions both perpendicular and parallel to the flow.

Funding acknowledgment: NSERC

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MS4 / 300

## Dissolution and swelling in porous media

**Authors:** André F. V. Matias<sup>1</sup> ; Rodrigo C. V. Coelho<sup>1</sup> ; José S. Andrade Jr.<sup>2</sup> ; Nuno A. M. Araújo<sup>1</sup>

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Transport in porous materials is a problem of relevance for several real-life applications such as disintegration of pharmaceutical tablets [1], groundwater contamination [2], and oil extraction [3]. In several cases the fluid changes the medium, and these changes are expected to feedback into the fluid flow. Examples of these changes are: i) erosion; ii) swelling; and iii) dissolution of solute. In a previous work, we focused on studying the dynamics of a porous medium that swells and erodes and showed that swelling can greatly impact the erosion of a porous medium [4]. Here, we study the competition between swelling and dissolution. We consider a porous medium composed of compacted non-overlapping spheres of size dispersion 5%. We use the Lattice-Boltzmann Method to resolve the fluid flow coupled to an advection-diffusion equation for the solute, to obtain the velocity field and solute concentration. The fluid flows due to an imposed pressure drop. On the surface of each sphere there is a flux of solute that depends on the solute concentration gradient and on the solid dissolution mass transfer coefficient [5]. The implementation of the sphere swelling is based on the discretization of an empirical law [6] consisting of an exponential increase of the sphere volume. Swelling has two competing effects on the solute transport: i) swelling decreases the average velocity of the fluid which causes a decrease on the solute throughput; and ii) swelling causes an increase in the surface area of the porous medium which in turn enhances solute dissolution. We investigate the impact of this competition on the extracted solute over time and determine an empirical equation that describes the extracted solute concentration.

**Time Block Preference:**

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## **Does the imaging domain size matter in modeling the permeability of bioclogged porous media inside a microfluidic channel with evolving biofilms?**

**Authors:** Shahab Karimifard<sup>1</sup> ; Xu Li<sup>1</sup> ; Yusong Li<sup>1</sup>

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This study integrates mathematical modeling and microfluidic experiments to study the impacts of imaging domain size on determining the permeability of porous media with evolving biofilm ratios. *E. coli* biofilms were grown to three biofilm ratios: low (2.7%), intermediate (17.6%), and high (55.2%) inside a microfluidic channel packed with a single layer of glass beads. Two-dimensional biofilm geometries in the porous space were extracted by digitizing confocal images. The permeability of the bioclogged porous media was estimated by solving the Navier-Stokes equations for flow in the pore spaces and a Forchheimer-corrected version of the Brinkman equation for flow inside biofilms using COMSOL. To evaluate the effect of modeling domain sizes on the estimation of the permeability, we simulated water flow in the bioclogged porous media using three smaller domain sizes (i.e., 1.5 mm × 1.5 mm, 2.5 mm × 2.5 mm, and 3.5 mm × 3.5 mm), in addition to the original domain size of 5 mm × 5.6 mm. We randomly selected five different porous medium areas for each domain size to conduct the simulation. In these simulations, biofilm porosity was assumed to be constant (0.6), and a range of biofilm permeability, including 10<sup>-9</sup> m<sup>2</sup>, 10<sup>-12</sup> m<sup>2</sup>, 10<sup>-15</sup> m<sup>2</sup>, and impermeable, was considered. We found that the modeling domain size was very important to estimate the permeability of bioclogged porous media, particularly when the biofilm ratio was low. Although the size of the modeling domain was found to be essential in estimating the permeability of lower biofilm levels, smaller domain sizes can be acceptable when biofilm structures are well developed.

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## Droplet absorption into thin layers of hydrogel

**Authors:** Merlin A. Etzold<sup>1</sup> ; George T. Fortune<sup>2</sup> ; Stuart B. Dalziel<sup>2</sup> ; Julien R. Landel<sup>3</sup> ; M. Grae Worster<sup>1</sup>

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Some cross-linked polymers, such as hydrogels, can absorb large quantities of solvents whilst undergoing a large change in volume. These chemically driven flows lead to a strong deformation of the polymer. In our experiments, we place a single droplet of water on a thin layer of strongly swelling polymer. Within minutes, a strongly swollen, very localised blister with a patterned surface forms. Over the next few hours, the pattern vanishes and the blister spreads radially whilst significant swelling remains.

We show that this process is driven by transport of solvent within the polymer and within the vapour contained in the surrounding gas phase. We also show how these two transport phenomena can be experimentally separated to enable the study of the transport within the polymer alone. The long-time dynamics of transport within the polymer is compared against a linear poroelastic model and a poroelastic model with porosity-dependent permeability which agrees well with the observed kinetics and blister shape.

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## Droplet formation, growth and detachment on the interface of a coupled free flow – porous medium system

**Author:** Maziar Veyskarami<sup>None</sup>

**Co-authors:** Rainer Helmig<sup>1</sup> ; Cynthia Michalkowski ; Carina Bringedal

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Interaction between free flow and porous medium is of great importance in various applications which is controlled by the interface between two domains. Since emerging a droplet on the interface significantly alters interface properties, it consequently has a considerable influence on coupling condition between free flow and porous medium. An interface including droplet not only handles exchange between free flow and porous medium, but also stores mass and energy [1]. Such an interface should also be able to describe the droplet behavior for instance formation, growth and detachment.

In order to better approximate the surface driven processes at the interface between the porous and the free flow, we use a pore network model [2, 3]. Here, the respective droplets are discretely approximated. Thus, the main processes such as the growth of the droplets and the detachment can be captured. Droplet detachment is captured by calculating the free flow forces on the droplet surface and the retention force, which results from the change in the contact angle of the droplet

along its contact line with the solid surface and the interfacial tension between two immiscible fluids. Selected examples are used to discuss the interaction behavior between free flow, porous medium and the formation and detachment of droplets.

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MS7 / 15

## Drying of capillary porous media simulated by coupling of continuum model and pore network model

**Authors:** Xiang Lu<sup>None</sup> ; Evangelos Tsotsas<sup>1</sup> ; Abdolreza Kharaghani<sup>2</sup>

<sup>1</sup> *Otto von Guericke University Magdeburg, Germany*

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Drying of porous media is traditionally described by macroscopic continuum models. In this frame, the partially-saturated porous medium is treated as homogeneous continuum and the fluid transport is driven by gradients of spatially-averaged quantities (such as moisture content) and controlled by non-linear (effective) parameters (such as moisture transport coefficient). The boundary conditions required to solve the continuum models are often specified either at the drying medium surface or at the drying front (i.e. the interface between the unsaturated and dry zones). The vapor pressure at the medium surface is often correlated to global or local moisture content using empirical expressions and the drying front velocity is determined from experimental observations. Such boundary conditions for coupling the internal and external transfer can be questionable. In this work, we recall an isothermal version of the broadly accepted macroscopic continuum model for drying porous media, and we impose flux boundary conditions at two interfaces, i.e., at the interface between the (gas-side) boundary layer and the (medium-side) dry region, as well as the interface between the dry and unsaturated regions which evolves freely during drying. Local relative humidity, local saturation as well as local transport parameters are computed from mesoscopic pore network simulations. This dataset is then employed to compute fluxes that couple the internal and external transfer in the continuum model. Decisive advantages of this approach over the classical method are that the continuity of the mass flux at the drying front and the porous medium surface is ensured and that the continuum model parameters are computed directly from pore network simulations – no need for any empirical correlation.

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## Drying of cellulose studied by Nuclear Magnetic Resonance

**Authors:** Xiaoyan MA<sup>1</sup> ; Alban GOSSARD<sup>2</sup> ; philippe Coussot<sup>1</sup>

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Cellulose has a very large range of applications in many aspects, and the drying of cellulose are widely adopted in many industrial processes. The deformable property of cellulose fibers, along with water adsorption capacity, add complexity to its drying mechanisms. In this work, we study the global mass loss and the spatial evolution of the internal water content of cellulose during its convective drying. Two complimentary approaches were adopted for this objective: macroscopic drying manipulations and nuclear magnetic resonance (NMR) For cellulose slurry, different concentrations of water-cellulose suspensions are dried under constant convection boundary conditions. Two obvious regimes are observed, corresponding to constant drying rate and decreasing drying rate. Meanwhile, the Magnetic Resonance Imaging results present three stages during the whole process: firstly, free water extracted accompanied with shrinkage of structures; followed by a second stage of homogeneously desaturation of all the bulk water; these stages correspond to the constant drying rate period. The last stage is assumed to be the confined water extraction, during which a slightly further shrinkage is observed as well. Complimentary experiments are carried out starting the drying test from cellulose powder prepared at saturated relative humidity, in order to capture the drying mechanism for confined water (possibly bound water). The profiles of NMR signal intensity, which is equivalent to water content inside cellulose, evolve in time in a way which appears consistent with a process of diffusion of vapor all along the sample interior (down to its bottom), in contrast with drying processes with liquid present inside the sample.

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## Dynamic adsorption of CO<sub>2</sub> in shale organic pores using molecular dynamic simulation

**Author:** Jingru Zhang<sup>1</sup>

**Co-authors:** Yi Zhang<sup>1</sup> ; Lei Yuan<sup>1</sup>

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The technology of CCUS(carbon capture,utilization and storage) has great potential for development. It is of great significance for CS-ESGR (CO<sub>2</sub> sequestration and enhanced shale gas recovery) to study the dynamic adsorption characteristic of CO<sub>2</sub> in the organic pore of shale. Most studies analyze the adsorption efficiency and influencing factors at the level of results, while less attention is paid to the phenomena in dynamic processes. In this study, a shale organic pore model consisting of 1 nm and 4 nm micropores connected by 8 nm mesopores is established. And then, the dynamic process of CO<sub>2</sub> diffusion from 8 nm mesopores to micropores and adsorption is investigated by using MD(molecular dynamics) simulation method. On this basis, the effects that different pressures on the diffusion of CO<sub>2</sub> into micropores with different pore sizes and the adsorption dynamic process

are also investigated. It is found that different pore sizes lead to different density distribution, and the dynamic process of diffusion and adsorption occurs in the micropore with pore size of 1 nm at first. This is due to the stronger pore effect of 1 nm micropore, which enhances the adsorption of CO<sub>2</sub> with the organic pore surface. At low pressure, the adsorption amount in the 4nm pore is always larger than that in the 1nm pore. At high pressure, the adsorption amount in the 4nm pore is larger than that in the 1nm pore at the initial stage, but it tends to be close to that in the end. In addition, it is beneficial for the faster diffusion of CO<sub>2</sub> into the micropore and stronger adsorption with increasing pressure. As a result, the adsorption process fluctuates at a less degree and is more stable at high pressure, the dynamic time to reach adsorption equilibrium is also smaller. It is concluded that pore size has an obvious effect on adsorption at low pressure, which can be explained by spatial constraints and interaction enhancement. While pore size effect gradually diminishes and pressure effect increases at high pressure.

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MS7 / 638

## Dynamic coarsening for efficient simulation of geothermal energy applications

**Author:** Øystein Klemetsdal<sup>1</sup>

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Whereas extraction of hydrocarbons from the subsurface typically involves transport phenomena over large distances (e.g. in-between injection and production wells), transport of geothermal heat during extraction and storage is chiefly confined to the proximity of wells. This indicates significantly reduced computational efforts by considering only a region of interest around the wells. In this work, we investigate a dynamic coarsening approach that uses aggregation of cells in an underlying fine-scale geomodel to form a coarse representation with refinement only in regions of interest. The dynamic grid is constructed from a predefined set of nested partitions of the underlying fine grid, and constructed at each timestep based on a set of suitable indicators. The approach is highly flexible, since it applies to any underlying fine grid consisting of non-overlapping cells, and efficient, since properties of the dynamic grids can be computed in a preprocessing step.

We assess the method on a number of test cases, and compare and contrast the results to fine-scale simulations using different refinement indicators and coarsening strategies. All numerical experiments will be conducted using the newly developed geothermal module of the open-source MATLAB Reservoir Simulation Toolbox.

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## Dynamic imaging of the impacts of flow instabilities and rock heterogeneity on CO<sub>2</sub> plume migration

**Authors:** Mojtaba Seyyedi<sup>1</sup> ; Michael Clennell<sup>1</sup> ; Samuel Jackson<sup>1</sup>

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Flow instabilities such as gravity override and viscous fingering, as well as rock heterogeneity could impact the CO<sub>2</sub> plume migration during storage operations in underground formations. This consequently impacts the CO<sub>2</sub> storage capacity of formations. Although over the past decade a significant amount of work has been conducted on the topic of CO<sub>2</sub> storage in underground formations, the interplay between flow instabilities and rock heterogeneity and how much each could control the plume migration are not fully resolved. Current limitations in understanding are mostly due to the small dimensional size (1.5”) of the samples in the majority of reported laboratory experiments. This undermines the impact of flow instabilities on the gas front and can not fully capture large-scale rock heterogeneity.

To address this gap of knowledge, we conducted a series of fluid-flow experiments in meter-long 4” Bentheimer and Boise sandstone outcrop cores using a high-pressure core flooding rig equipped with a medical X-Ray CT scanner. The cores were initially saturated with a synthetic brine where the cores’ heterogeneity structures were identified by 3D image processing of the medical CT data. Brine-saturated cores were horizontally flooded with nitrogen, and their dynamic 3D flow patterns and fluid distributions were studied by analyzing captured 3D volume data sets. The results show that for the case of the Bentheimer core, which is much less heterogeneous compared to Boise, the plume migration is mostly controlled by buoyancy forces with heterogeneity-induced gas channeling occurring at the bottom side of the core. On the other hand, for the case of Boise, the rock structural heterogeneities led to stronger gas channeling which consequently reduced the vertical plume migration driven by buoyancy forces and improved the storage potential of the gas compared to homogenous cases. The results show that depending on the rock heterogeneity and heterogeneity direction, gas channeling could occur which could hinder the vertical CO<sub>2</sub> plume migration driven by buoyancy forces and improve the storage capacity of the storage site.

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## Dynamic mesh optimisation for geothermal reservoir modelling

**Authors:** Pablo Salinas<sup>None</sup> ; Geraldine Regnier<sup>1</sup> ; Carl Jacquemyn<sup>1</sup> ; Christopher C. Pain<sup>1</sup> ; Matthew D. Jackson<sup>1</sup>

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Numerical modelling of fluid flow and heat transport in geothermal reservoirs can be very challenging due to the need of modelling several length-scales simultaneously that control the flow behaviour. The length-scales to consider typically go from fractures (millimetre-scale) and wells (metre-scale) to facies architecture and faults (kilometre-scale). The usual approach for modelling geothermal reservoirs is to discretise the equations using the finite-volume method subdividing space onto a

fixed, structured mesh. However, using a fixed mesh resolution across the entire model domain can be very computationally expensive, and prohibitive if the model must resolve many length-scales simultaneously. Moreover, large domains may be necessary as well to avoid boundary effects and to include the whole convective system hosting a particular reservoir.

In other areas of computational fluid dynamics, high fidelity solutions have been obtained at lower computational cost by use of dynamic mesh optimisation (DMO), in which the resolution and geometry of the mesh varies during a simulation to minimize an error metric for one or more solution fields of interest such as pressure or velocity. DMO varies the mesh resolution such that higher resolution is used in parts of the domain where the solution is complex, and lower resolution is used elsewhere.

Here we report an efficient method to apply dynamic adaptive mesh optimisation (DMO) to model geothermal reservoirs. The method reported here uses a surface-based representation of all geological heterogeneity that should be captured in the model. In surface-based geologic modelling (SBGM), all geological heterogeneities of interest are represented by surfaces: these surfaces may capture faults, fractures, stratigraphic surfaces, etc. The surfaces define rock volumes which we term ‘geologic domains’. These domains have constant petrophysical properties, or simple, mathematically defined trends such as upwards or downwards increases in permeability. When simulating, the mesh dynamically adapts to optimise the representation of key solutions metrics of interest, but the surface architecture is preserved.

We demonstrate the method using a number of example problems including wells and high permeable fractured media. These heterogeneous test cases represent common reservoir scenarios that can be difficult to represent in conventional geothermal reservoir modelling workflows. We focus here on thermal-hydrological (TH) processes in the low enthalpy geothermal systems that are used to source and store heat in many different locations around the world. Another advantage of our approach is that well trajectories are accurately represented as the mesh conforms to the well-path. We show that more accurate results are obtained, while modelling simultaneously several length-scales, at lower computational cost as compared to conventional fixed mesh approaches.

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## Dynamic pore-network modeling of coupled compositional flow and phase change dynamics in porous media

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Compositional flow and phase change dynamics in porous media play a central role in many industrial and geoscience applications including fuel cells, geologic CO<sub>2</sub> sequestration, and hydrocarbon production. Though the interplay between transient two-phase flow and phase change dynamics is of critical important, it remains not well understood limited by computational challenges especially for direct numerical simulations. We develop a novel dynamic pore-network model to simulate two-phase compositional flow and phase change dynamics in complex pore structures. The model formulation couples a thermodynamic phase-equilibrium model for multicomponent fluids in each individual pore to a dynamic pore-network model for two-phase compositional flow. The new coupled modeling framework allows us to investigate the interactions between compositional



flow dynamics and phase change dynamics in highly disordered pore structures extracted from 3D digital images of rock samples. A series of example simulations of two-phase displacements show that phase change (evaporation and condensation) can suppress fingering patterns generated during invasion.

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MS6-A / 78

## Dynamics of Water and Gas Injection in an Oil-Wet Reservoir Rock at subsurface conditions: A Pore-Scale Synchrotron X-ray Imaging Study

**Author:** Abdulla Alhosani<sup>1</sup>

**Co-authors:** Alessio Scanziani<sup>1</sup>; Qingyang Lin<sup>1</sup>; Ahmed Selem; Amer Alhamadi<sup>1</sup>; Sajjad Foroughi<sup>2</sup>; Branko Bijeljic<sup>3</sup>; Martin Blunt<sup>1</sup>

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Understanding the pore-scale fluid dynamics occurring during multiphase flow in porous media is important for the design of many applications including subsurface carbon dioxide storage, microfluidic devices, membrane fuel cells, and packed bed chemical reactors. To investigate the displacement dynamics of two- and three-phase flow in a hydrophobic porous medium, we use synchrotron X-ray microtomography to image the flow of water and gas in an oil-wet reservoir rock at high pressure and temperature (8 MPa and 60 °C).

After altering the wettability of the rock surface, towards oil-wet conditions, in a process known as ageing, water is injected at a very low flow rate (0.15 µL/min) in the oil-filled rock which is simultaneously imaged every 70 s to track the advance of the water front. Gas is then injected in the system at the same flow rate and images are acquired every 74 s. The use of fast synchrotron imaging with a high spatial resolution (3.5 µm) allows us to examine, in situ, (i) wettability and displacement contact angles, (ii) invasion patterns (pore-filling order), (iii) displacement events, (iv) fluid connectivity, and (v) change in Minkowski functionals – fluid saturations, specific interfacial areas, and curvatures.

During water injection, the displacement of oil by water is a drainage-like process, where water advances as a connected front displacing oil in the center of the pores, confining the oil to wetting layers. The displacement is an invasion percolation process, where throats, fill in order of size, with the largest available throats filled first, indicating that the displacement in our heterogeneous rock is predominantly size controlled. Furthermore, we observe drainage associated pore-filling dynamics including Haines jumps and snap-off events during water injection. Haines jumps occur on single- and/or multiple-pore levels accompanied by the rearrangement of water in the pore space to allow the fast filling. Snap-off events are observed both locally and distally with trapped water ganglia reconnecting as the water injection proceeds.

During the subsequent gas injection, gas invades the rock in a unique pattern, where it progresses through the pore space in the form of disconnected clusters mediated by double and multiple displacement events. Gas advances in a process we call three-phase Haines jumps, during which gas re-arranges its configuration in the pore space, retracting from some regions to enable the rapid filling of multiple pores. Nevertheless, unlike the two-phase water injection, the gas retraction leads to a permanent disconnection of gas ganglia, which do not reconnect as gas injection proceeds. We

observe, in situ, the direct displacement of oil and water by gas as well as gas–oil–water double displacement. The wettability order is oil–gas–water from most to least wetting, indicating that the rock surface is strongly oil-wet. Furthermore, quantifying the evolution of Minkowski functionals implied well-connected oil and water phases, while the gas connectivity decreased as gas was broken up into discrete clusters during injection.

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## **Dynamics of organic pore evolution in shale under varying thermal and oxygen environments**

**Authors:** Tuli Bakshi<sup>1</sup> ; Debanjan Chandra<sup>1</sup> ; Vikram Vishal<sup>1</sup>

<sup>1</sup> *IIT Bombay*

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The high heterogeneity of shale is a deterrent in the accurate assessment of reservoir characteristics, making gas exploitation a challenging task. Besides being a nearly impermeable permeable reservoir type, shale has a complex pore network exhibited by various pore types and pore-size distributions that influence gas storage and transport in the shale matrix [1,2]. Gas in shale is stored as (1) free gas in pores and fractures, (2) adsorbed gas inside organic matter and clay pores; and (3) dissolved gas in water [3,4]. Micropores, present in organic matter and clay minerals, primarily adsorb gas owing to their large specific surface area and more significant adsorption potential in small pores [3,4]. Temperature plays a vital role in modifying shale pore characteristics. Thermally mature shales have larger micropore volume and higher gas sorption capacity than immature shales [5]. With increasing temperature, the thermal cracking of kerogen takes place, leading to a restructuring of organic pores [6]. Although studies exploring the pore structure changes in oil shales through inert heating are plenty, such research rarely exists in the field of gas shale. Due to the probable harmful environmental effect of hydraulic fracturing, more research is being done worldwide to develop a greener solution to improve shale gas resource exploitation [7]. New studies suggest combustion as an alternative technique for porosity enhancement as the process eliminates kerogen and organic matter resulting in higher gas recovery from shale [8].

So far, studies on Indian shales have been analyzing overall pore characteristics and their relation to the organic matter properties and gas adsorption capacities [4,5,9,10]. However, very few works detail the influence of increasing temperature on Indian shale pore, when the thermal treatment takes place in oxygen. Hence, the prime focus of this study is to assess the dynamics of organic pore development in shale when it is combusted in the presence of oxygen. The pore attributes were estimated using low-pressure N<sub>2</sub> and CO<sub>2</sub> adsorption (LPGA) at each temperature interval, further supported by high-resolution microscopy. The temperature of 300°C is taken as a maximum as a further rise in the temperatures might alter clay, and kerogen's fundamental characteristics in shales [11].

The aliphatic hydrocarbon stretching bands of kerogens, identified from FTIR study, at 2920 cm<sup>-1</sup> and 2850 cm<sup>-1</sup> display a reduction of almost 13% in the aliphaticity from 100°C to 300°C. SEM images also confirm the growing connectivity of organic micro-pores with gradual temperature rise. LPGA analysis confirms the appearance of newer micropores with rising temperature and formation of larger pores at 300°C. However, when samples were heated in an inert environment, changes in pore characteristics occur differently. Oxidic heating causes a noticeable increase in the surface area and pore volume (almost 70-80%). Along with that, the pore size distribution peaks become sharper and of higher magnitude. But when the samples were heated in the absence of oxygen, pore-blocking occurs due to the generation and solidification of bitumen, resulting in a reduction of surface area and pore volume almost up to 30%.

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**Poster + / 697****Dynamics of unsaturated flow in fracture networks: impact of local splitting behavior at the intersection****Authors:** Zhibing Yang<sup>1</sup> ; song xue<sup>2</sup> ; Ran Hu<sup>1</sup> ; Yi-Feng Chen<sup>1</sup><sup>1</sup> Wuhan University<sup>2</sup> wuhan university**Corresponding Authors:** csyfchen@whu.edu.cn, zbyang@whu.edu.cn, whuran@whu.edu.cn, 125930515@qq.com

Understanding the physical mechanisms of unsaturated flow in fractured vadose zone at different scales is an important for subsurface hydrology. Here we develop a network model to study infiltration in unsaturated fracture networks. We consider an idealized fracture network composed of a series of Y-shaped intersections. At each intersection, liquid storage/release and splitting/convergence behaviors are modeled according to local splitting relationships obtained from detailed laboratory work and numerical simulations. By varying the splitting relationships, we systematically investigate the influence of local flow behaviors on large scale flow structures. We show that when the water tends to split equally at the intersection, a divergent flow structure forms in the network. Conversely, preferential pathways emerge in case of unequal splitting. We find that an avalanche infiltration mode, i.e., sudden release of a large amount of water from the network, emerges spontaneously. This flow mode is modulated by the local splitting behavior. The pathways of preferential flow is controlled by the liquid volume triggered by avalanches and the network structure.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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## EPISODIC EXTREME RAINFALL EVENTS DRIVE GROUNDWATER RECHARGE IN ARID ZONE ENVIRONMENTS OF CENTRAL AUSTRALIA

**Author:** Dirk Mallants<sup>1</sup>

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To improve estimates of long-term average groundwater recharge in data sparse arid regions, we combined a numerical multi-model approach with century-long time series of meteorological data and site-specific regolith hydraulic properties. The numerical model was set up in the vadose zone simulator HYDRUS-1D for a bare soil and a Mulga (*Acacia aneura*) savanna-type soil in central Australia. Grain-size analysis from regolith cores were used to generate contiguous 12-m deep profiles of hydraulic properties by means of pedotransfer functions. In order to account for conceptual model uncertainty in generated hydraulic properties that are required as input for the physically based soil-water balance model, eleven pedotransfer functions were applied. Three types of PTFs were used: point estimation (Bruand et al. (1994), Canarache (1993), Gupta and Larson (1979), Hall et al. (1977), Petersen et al. (1968), Varallyay et al. (1982)), parametric (Vereecken et al. (1989), Wösten et al. (1999)), and class PTFs (Meyer et al. (1997), Schaap et al. (2001), Wösten et al. (1999)). Climate data from three stations were used to account for spatial heterogeneity in local climate of the Ti Tree Basin case study area. Analysis of simulated water fluxes in the vadose zone indicated that only rainfall events of more than 200 mm resulted in noticeable fluxes at the bottom of the 12-m deep regolith. Recharge events were linked to extreme rainfall associated with monsoonal cyclones. Based on the 130-year climate records, long-term average recharge for the savanna-type vegetation ranged from 4.3 to 7.4 mm/a across the three climate stations, with an overall mean of 4.6 mm/a. The bare soil had an overall mean recharge of 29.5 mm/a, ranging from 23.5 to 35.8 mm/a depending on climate station. Results from this study yield a better understanding of the highly episodic and spatially variable recharge in arid and semi-arid environments and is critical input to sustainably manage groundwater resources.

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## EUTROPHICATION CONTROL TREATMENTS AND SEDIMENT POROSITY

**Authors:** Anne M. Hansen<sup>1</sup> ; DAngelo Sandoval-Chacón<sup>2</sup> ; Vanessa G. Moreno-Ayala<sup>1</sup>

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Different land uses and wastewater discharges from point and diffuse emission sources result in accumulation of nutrients, or eutrophication of lakes and reservoirs, and water quality not meeting standards for different uses. Consequently, 70% of the approximately 300 lentic water bodies monitored in Mexico are in a eutrophic or hypereutrophic state [1]. Different methods have been proposed for the rehabilitation of eutrophic water bodies, where the following stand out (1) hypolimnetic oxygenation systems (HOS), where organic matter is expected to be more readily degraded and iron oxyhydroxides are formed that can immobilize nutrients, and (2) application of a phosphorus selective adsorbent (Phoslock) in water and sediment, that restrains this limiting nutrient [2]. The effectiveness of these treatments depends on the accessibility of these amendments to surfaces inside the porous structure of sediments, and the question arises if there are structural changes due to the application of these methods? We evaluated how these treatments affected mineralization rates of organic matter, immobilization of phosphorus, changes in pore volumes, distribution of pore areas in the sediment. The sediment had a predominant pore size of  $5.2 \pm 1.5$  nm with an initial specific surface area of 46 m<sup>2</sup>/g, which increased to 58 m<sup>2</sup>/g with the HOS treatment and decreased to 41 m<sup>2</sup>/g or less with the Phoslock and combined treatments and without treatment (Control). The pore volume remained at  $0.09 \pm 0.01$  cm<sup>3</sup>/g with no variation between treatments. It was determined that the mineralization rate of organic matter was higher in the Control reactor (44% of the organic matter in 220d) and lower in the reactors with treatments ( $32 \pm 5\%$  of the organic matter). The treatments did therefore not affect the pore volume or diameter. The different mineralization reactions identified through ion release and depletions during the treatments, were related to variations in surface areas of the sediment. The financial supports from IMTA (TH1913.1 and TH2012.1), Conacyt (scholarship- CVU 780094) and the Office of International Affairs and External Cooperation of the University of Costa Rica, are acknowledged.

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## **EVALUATION OF SURFACTANT AND FOAM PROCESSES FOR IN-SITU NAPL REMEDIATION IN A MILITARY BASE, SOUTH KOREA**

**Authors:** Hazem Fleifel<sup>1</sup> ; Gyu Sang Lee<sup>2</sup> ; SEUNG Kam<sup>1</sup>

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## Introduction

Surfactant and foam processes have been widely used in enhanced oil recovery from the petroleum-bearing geological formations [1, 2] and in-situ subsurface remediation from shallow formation and aquifer [3, 4].

This study investigates the potential of using surfactant and foam processes for the in-situ remediation of shallow subsurface NAPL phases within a field in a US/Korea military base, South Korea. It consists of two major components: the first is a history matching of surfactant enhanced aquifer remediation treatment and the second is a prediction of follow-up foam injection treatment. The site has a 5 m x 5 m treatment area with 3 m depth with 3 injection wells and 3 extraction wells.

## Results

**Surfactant treatment:** Over 10-days surfactant treatment exhibits a partial success in terms of NAPL removal. The relatively higher-permeability area contacted by the surfactant chemicals shows a mobilization of NAPL phases because of a reduced level of capillary trapping (i.e., low dimensionless capillary number). It is the area with relatively lower-permeability values, however, that prevents a successful sweep from occurring. History matching from simulations shows why such an early breakthrough happens in some extraction wells, and what roles the subsurface heterogeneity plays in overall in-situ treatment with surfactant solution.

**Foam treatment:** A foam treatment, proposed as a potential follow-up action, is evaluated see if how foam can overcome subsurface heterogeneity. The outcome seems very promising such that foam can improve the sweep and increase the recovery factor over 80 - 90%. The final results are shown to vary with foam strengths as summarized by using a sensitivity analysis. Foam field test is designed in the near future.

## Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

[1] S.I. Kam and W.R. Rossen. A Model for Foam Generation in Homogeneous Media, SPE Journal, 417-425, (2003).

[2] M. Izadi and S.I. Kam. Investigating Supercritical CO<sub>2</sub> Foam Propagation Distance: Conversion from Strong Foam to Weak Foam vs. Gravity Segregation, Transport in Porous Media, DOI: 10.1007/s11242-018-1125-z, (2019).

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Poster + / 38

# EXPERIMENTALLY VALIDATED SIMULATION OF STRAIN-INDUCED BATTERY AGING

**Authors:** Ilona Glatt<sup>1</sup> ; Nils Wenzler<sup>2</sup> ; Mathias Fingerle<sup>1</sup> ; Raphael Zahn<sup>2</sup>

**Co-authors:** Fabian Biebl<sup>3</sup> ; Erik Glatt ; Sven Linden<sup>1</sup> ; Sebastian Rief<sup>1</sup> ; Andreas Wiegmann<sup>1</sup> ; Vanessa Wood<sup>2</sup>

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During cycling, volumetric changes of the active material induce stresses on the micro- and macro-scale, leading to cracks and delamination, and deformation of the inactive layers and the casing [1]. The altered microstructure is said to “age” and it suffers from capacity loss and damaging effects like lithium-plating [2]. The quantitative simulation of this battery aging on a microstructural level is now jointly pursued by Math2Market and the MaDE group of Prof. Vanessa Wood (ETH Zürich) in the framework of the EU-project “SOLVED!”.

Our approach is to analyze NMC cathode and graphite anode microstructures via 3D in-vivo tomography and electrochemical characterization [3]. The experimental data is used to validate the degradation simulations in which local volumetric changes and damage due to lithium intercalation on the microscale are linked to the local Li-ion concentration in the active material and its mechanical deformation. In a dynamic process, the altered microstructure is considered for each charging and discharging step. In this way, the influence of structural changes on the electronic and ionic transport processes and on the macroscopic performance of the cell is digitally predicted and monitored.

The usage of reliable quantitative simulations allows for the timesaving and streamlined finding of new prototype materials with superior lifetime and performance. This unique workflow represents a new efficient, state-of-the-art approach to digital R&D material design for energy materials in e-mobility and energy storage.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

[1] Quantification and modeling of mechanical degradation in lithium-ion batteries based on nanoscale imaging. S. Müller, P. Pietsch, B.-E. Brandt, P. Baade, V. De Andrade, F. De Carlo, V. Wood, 2018, Nature Communications, DOI: 10.1038/s41467-018-04477-1

[2] Investigation on the temperature dependence of lithium plating in commercial Li-ion batteries. M. A. Cabañero et al., Electrochimica Acta 171, 1217–1228 (2017).

[3] X-Ray Tomography for Lithium-ion Battery Research: A Practical Guide. P. Pietsch and V. Wood, Annu. Rev. Mater. Res., 2017, 47, 451–479 **Acceptance of Terms and Conditions:**

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MS6-A / 118

## Effect of Pore-Scale Wettability Distribution Patterns on Fluid Connectivity

**Authors:** Omid Shahrokhi<sup>1</sup> ; Amir Jahanbakhsh<sup>1</sup> ; Krystian Wlodarczyk<sup>1</sup> ; Duncan P. Hand<sup>1</sup> ; Mercedes Maroto-Valer<sup>1</sup>

<sup>1</sup> Heriot-Watt University

**Corresponding Authors:** d.p.hand@hw.ac.uk, m.maroto-valer@hw.ac.uk, k.l.wlodarczyk@hw.ac.uk, o.shahrokhi@hw.ac.uk, a.jahanbakhsh@hw.ac.uk

Multiphase flow is ubiquitous in natural porous media, synthetic membranes like fuel cells and microfluidics. The wetting state of these materials is one of the key controlling parameters of fluid distribution and it dictates trapping behaviour of each phase. At pore-scale, contact angle measurement by in-situ imaging of phase interfaces can explain phase trapping [1]. However, the spatial distribution of these micro-scale contact angles govern average trapping and flow dynamics at the continuum scale. This is especially critical for porous media with heterogeneous mineral distributions where significant changes in surface energy exist in different flow paths. The main challenge to upscale pore-scale wettability distributions to Darcy scale is the non-uniqueness of the solutions (e.g. capillary and relative permeability curves) because of infinite pore size and wettability distribution combinations. Defining a parameter to classify different spatial distributions can be a step toward reducing the degree of freedom for possible dynamics.

Accordingly, this work aims to understand the effect of different spatial wettability distributions on phase trapping and fluid connectivity patterns. We have used a set of spherical glass bead packs to

isolate the effect of pore size distribution from wettability distribution on phase trapping by altering packing methods of silanized glass beads. The produced glass bead packs with different wettability distributions represent common wettabilities of rock types reported in the literature [2–4]. To reduce the uncertainty of measuring contact angles by image analysis two approaches were taken, namely selecting glass beads with negligible surface roughness values (MoSci Class VI, 250 $\mu$ m) and avoiding very low contact angles. The surface roughness of the glass bead samples was measured with Alicona Surface Profilometer. The measured values (arithmetical mean height Sa=100-200nm) are below the effective pixel size of the Nikon MicroCT XT H 225 rig (3 $\mu$ m) used for in-situ imaging. Moreover, the glass beads were treated such that contact angles are above 20° to avoid errors involved with small contact angle measurements. The flow tests through the packed glass beads start by injecting 20 pore volumes (PV) of doped brine to displace air to ensure no further changes in trapped phase distribution during microCT imaging. This was followed by air (20PV) and another water injection period (20 PV each).

The images of fluid distribution in the glass bead packs were analysed with a programmed script for Avizo visualization software and the spatial trapping patterns and quantities are discussed in terms of wetting correlation length  $\xi$ . Generally, we observed higher trapping but more uniformly dispersed non-wetting phase for higher wettability heterogeneity at pore-scale (lower  $\xi$ ). However,  $\xi$  values did not fully explain trapping distribution when they approached Darcy scale lengths. The result of this work is a step toward defining a parameter to classify different spatial wettability distributions.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

#### References

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MS16 / 464

## Effect of The Relative Humidity on The Porosity of PEM Fuel Cell Catalyst Layers

**Authors:** Karrar Alofari<sup>None</sup> ; Ezequiel Médiçi<sup>1</sup> ; Jeffrey Allen<sup>2</sup>

<sup>1</sup> *Michigan Technological University*

<sup>2</sup> *Michigan Technological University*

**Corresponding Authors:** jstallen@mtu.edu, efmedici@mtu.edu, ktalofar@mtu.edu

The anode and cathode catalyst layers of proton-exchange membrane fuel cell, a thin porous media of approximately 10 $\mu$ m thickness and 50% porosity, have a complex solid structure composed by a support matrix to conduct electrons and provide structural integrity, ionomer films to conduct protons, open pores to transport gases, vapor, and liquid water; and dispersed catalyst particles, typical Platinum. The behavior of the ionomer films adds complexity to the solid phase as it can retain water which causes swelling and therefore changing the porosity and the mass transport behavior for both gases and condensed liquid water. In this study, an experimental setup is used to investigate mass transport in catalyst layers at different relative humidity (RH). To decouple swelling



and liquid water percolation phenomenon, an ionomer swelling neutral liquid, fluorinert FC-3283, is utilized as the working liquid. The RH is then controlled by changing the water vapor content in the gas phase. The experimental results show that when fluorinert is injected into the catalyst layer at a constant flow rate, as the RH in the gas phase increases the injection pressure for both the liquid and gas increases due to swelling and reduction in porosity. Paradoxically, at high RH it takes a longer time to reach bubble point than at low RH. This unexpected observation could be a key feature in understanding the complex relationship between mass transport, swelling, and porosity in the catalyst layers.

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Poster + / 72

## Effect of Viscosity Contrast on Miscible Rayleigh-Taylor Convection in Porous Media

**Authors:** Nasser Sabet<sup>1</sup> ; Hassan Hassanzadeh<sup>2</sup> ; Anne De Wit<sup>3</sup> ; Jalal Abedi<sup>2</sup>

<sup>1</sup> *Research Assistant*

<sup>2</sup> *University of Calgary*

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Rayleigh-Taylor (RT) convection is a buoyancy-driven instability arising when a denser fluid overlies a less dense one in a gravitational field. In this work, we study RT instability in porous media where the denser fluid on the top is also more viscous. We perform high-resolution numerical simulations through hybridization of pseudo-spectral and compact finite difference methods. Using our simulations, we study RT instability for a wide range of viscosity ratios, up to 3000. For the first time, we find that there is a critical viscosity ratio beyond which the up-down symmetry of fingers breaks down such that the downward fingers become more extended than upward fingers as the viscosity ratio increases. In this regard, we develop universal scaling relations for the spreading rate of fluids and the convective mass flux at the interface. Finally, we introduce a new secondary fingering instability and verify our finding by comparing the results with a set of previous experiments. Our study provides a more realistic understanding of miscible Rayleigh-Taylor convection in porous media by accounting for the viscosity variations.

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MS6-B / 295

## Effect of Wettability on Immiscible Liquid Displacement in 2D and 3D Porous Media

**Authors:** Debora do Nascimento<sup>1</sup> ; Jorge Avendano<sup>1</sup> ; Nicolle Lima<sup>1</sup> ; Marcio Carvalho<sup>1</sup>

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Wettability has a dramatic impact on fluid displacement in porous media. The pore level physics of one liquid being displaced by another is a strong function of the wetting characteristics of the channel walls. However, the quantification of the effect is still not clear. Conflicting data have shown that in some oil displacement experiments in rocks, the volume of trapped oil falls as the porous media becomes less water-wet, while in some microfluidic experiments the volume of residual oil is higher in oil-wet media. The reasons for this discrepancy are not fully understood. In this study, we visualize and analyze oil displacement by water injection in 2D and 3D model porous media with different wettability. The resulting oil ganglia size distribution at the end of water injection was quantified by image processing.

Detailed information on the trapped ganglia size and morphology is presented at different flow conditions. The results show that the displacement efficiency varies with capillary number; at low capillary number, the oil-wet porous media, the displacement front was more uniform and the final volume of remaining oil was smaller, with a much smaller number of large oil ganglia and a larger number of small oil ganglia, when compared to the water-wet media. At high capillary number, the behavior is the opposite.

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MS6-B / 557

## Effect of grain circularity on the temporal evolution of interfacial area

**Authors:** Fizza Zahid<sup>1</sup> ; Jeffrey Cunningham<sup>1</sup>

<sup>1</sup> University of South Florida

**Corresponding Authors:** cunning@usf.edu, fizzazahid@usf.edu

Multi-phase flow is controlled by the pore geometry of the porous domain, which is formed by the grain morphology. Grain morphology not only influences fluid behavior and transport but also affects the development of interfacial area over time. One quantitative measure of grain morphology is circularity, i.e., how closely a grain resembles a perfect sphere. The objective of this work is to quantify how grain circularity affects the temporal development of interfacial area during multi-phase flow through porous media. A multi-phase lattice Boltzmann method (Guntensen et al., 1991; Reis and Phillips, 2007) is used to simulate oil-water drainage and imbibition in an ensemble of two-dimensional porous media samples (Mollon and Zhao, 2012). We conducted multi-phase simulations on 3 groups of porous media which involved: 20 realizations of spherical grain shapes, 20 realizations of intermediate grain shape, and 20 realizations of elongated grain shapes. Interfacial area was periodically monitored during drainage and imbibition simulations in 60 samples, until the samples acquired steady-state fluid saturations. During drainage and imbibition, the interfacial area increases with time, acquires a peak value, and then decreases before reaching a plateau at steady-state. All three groups of porous media showed the same temporal trend, with no major differences. However, the domains with highly circular groups showed an average 16 percent residual water saturation at the end of drainage, while only a 10 percent average residual water saturation was observed in the other two groups. The results indicate that grain circularity does not strongly affect the temporal evolution of interfacial area but influences the residual fluid volumes in the system. This implies that in case of oil spills in groundwater, spherical grains would be expected to have more water

residual than an elongated grain system. Therefore, the results of this work can help understand oil contamination in groundwater and improve soil remediation efforts.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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Mollon, G., & Zhao, J. (2012). Fourier–Voronoi-based generation of realistic samples for discrete modelling of granular materials. *Granular Matter*, 14(5), 621-638. **Acceptance of Terms and Conditions:**

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MS6-B / 148

## Effect of grain shape on quasi-static fluid-fluid displacement in porous media

**Authors:** Zhongzheng Wang<sup>1</sup> ; Jean-Michel Pereira<sup>2</sup> ; Yixiang Gan<sup>1</sup>

<sup>1</sup> *The University of Sydney*

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We study how grain shapes impact multiphase flow in porous media in the quasi-static regime. An extended pore-network model with interface tracking algorithm is presented, which considers meniscus pinning at sharp edges of grain. Our results show that the effective contact angle distribution during displacement widens as the grain becomes more angular, which consequently modifies the macroscopic fluid invasion morphology. By analyzing various characteristic metrics during displacement, including capillary pressure signal, Haines jump size distribution, and fractal dimension, our results highlight the profound influence of particle shape on the multiphase flow.

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## Effect of non-uniform passive advection on A+B->C radial reaction-diffusion fronts

**Authors:** Alessandro Comolli<sup>1</sup> ; Anne De Wit<sup>2</sup> ; Fabian Brau<sup>1</sup>

<sup>1</sup> *ULB - NLPC*

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The interplay between chemical and transport processes can give rise to complex reaction fronts dynamics, whose understanding is crucial in a wide variety of environmental, hydrological and biological processes, among others. An important class of reactions is  $A+B\rightarrow C$  processes, where A and B are two initially segregated miscible reactants that produce C upon contact. Depending on the nature of the reactants and on the transport processes that they undergo, this class of reaction describes a broad set of phenomena, including combustion, atmospheric reactions, calcium carbonate precipitation and more. Due to the complexity of the coupled chemical-hydrodynamic systems, theoretical studies generally deal with the particular case of reactants undergoing passive advection and molecular diffusion. A restricted number of different geometries have been studied, including uniform rectilinear [1], 2D radial [2] and 3D spherical [3] fronts. By symmetry considerations, these systems are effectively 1D.

Here, we consider a 3D axis-symmetric confined system in which a reactant A is injected radially into a sea of B and both species are transported by diffusion and passive non-uniform advection. The advective field  $v_r(r, z)$  describes a radial Poiseuille flow. We find that the front dynamics is defined by three distinct temporal regimes, which we characterize analytically and numerically. These are *i*) an early-time regime where the amount of mixing is small and the dynamics is transport-dominated, *ii*) a strongly non-linear transient regime and *iii*) a long-time regime that exhibits Taylor-like dispersion, for which the system dynamics is similar to the 2D radial case.

**Time Block Preference:**

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**Poster + / 373**

## Effect of pore geometry and contact angle on the capillary pressure and oil recovery factor in models of porous media

**Authors:** Afshin Davarpanah<sup>1</sup> ; Simon Cox<sup>1</sup>

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We model the displacement of oil from idealized porous media by simulating the quasi-static injection of gas into oil-filled channels with uniform cross-section under different wetting conditions.

We consider channels with triangular or rectangular cross-section that are initially filled with a single fluid (e.g. oil). A second, displacing, fluid (e.g. gas) is introduced at one end of the channel, first having to overcome the capillary entry pressure pce; we estimate pce based on the largest hemisphere that fits inside the cross-section of the channel.

The Surface Evolver software [1] is then used to simulate the invasion of the pore space by this second fluid. It allows us to find the shape of the interface with minimum surface energy separating the two fluids, for a given contact angle at which they meet the pore walls, and a highly-accurate measurement of the capillary pressure. By making small changes in the gas volume and repeating the minimization, we predict in a quasi-static manner the variation of capillary pressure during the displacement flow. As well as neglecting viscous losses, we assume that the effects of gravity are negligible (small Bond number, based on the usual pore size being small).

When the interface is far from the ends of the channel the flow reaches a steady state. In this regime we predict the oil recovery factor, i.e. the proportion of the first fluid that is displaced by the second. We show that in any channel:

- The capillary pressure decreases as the oil volume increases, for given contact angle;
- The capillary pressure decreases as the contact angle increases, for given oil volume;

and hence that the volume of oil that remains in the corners of the channel is greater for smaller contact angles, decreasing the recovery factor.

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MS16 / 144

## Effect of surfactants on liquid absorption into porous media

**Authors:** Helder Salvador<sup>1</sup> ; Daniel Turkenburg<sup>1</sup> ; Jeroen Schell<sup>1</sup> ; Nicolae Tomozeiu<sup>1</sup>

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Surfactants play an important role in nearly the entire inkjet process including dispersion stability, jetting, spreading and absorption into porous media. In this work we used two main methods to extract the absorption dynamics of water and surfactant mixtures into porous media, namely Automatic Scanner Absorptiometer and a pico Liter drop watcher setup. Combining both methodologies it was possible to get information about the dynamics of liquid absorption into porous media.

The aim of this work is to study the consequences of surfactants on the absorption behaviour into porous media. For that, we used as surfactant the Surfynol series (104, 440, 465, and 485) mixed with water at CMC value. We studied in detail the increase of the hydrophilic part of the surfactant and correlate that with the absorption behaviour. This is performed for uncoated media and for coated media with a very different polarity (Inkjet vs Offset)

We have concluded that the structure of paper has a substantial effect on the interaction behaviour. For coated media we have seen little influence of the surfactant on the absorption behaviour; however for uncoated media we could have a difference on the absorption rate up to an order of magnitude. Furthermore we concluded that increasing the hydrophilic behaviour of the surfactant leads to a lower absorption rate.

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Analysis of droplet spreading versus droplet absorption using ASA and pico-liter setup, Joep Sanders, 2021

Dynamics of fluid mixtures and nanoparticles during capillary suction, Cornelis Kuijpers, 2018

Dynamic behaviour of pl droplets on substrates, Helder Salvador, 2019

Surfynol surfactants, IMCD. <https://www.imcdus.com/en-us/products/surfynol-surfactants> **Acceptance**

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MS8 / 593

## Effective Transport Parameters of Porous Media from Microstructure Images.

**Authors:** Lukas Maier<sup>1</sup> ; Joern Henning Matthies<sup>1</sup> ; Ulrich Niekén<sup>2</sup>

<sup>1</sup> *University of Stuttgart, Institute of Chemical Process Engineering*

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Transport in porous media is central in chemical engineering. Effective transport properties are required for evaluating and improving many processes and applications, typical example are catalysts, or porous membranes in separation processes. A widely used model to describe transport in porous media is the Dusty-gas model. This model accounts for permeation, Knudsen-diffusion and binary diffusion. The model parameters are commonly determined from experiments, for instance, performed in a Wicke-Kallenbach cell [1]. The parameters derived in this way are spatially averaged effective parameters.

In this contribution we present an approach to calculate transport parameters of the Dusty-Gas model from a cross sectional image of a porous material. This reduces the currently large experimental effort, since only once a visualization of the microstructure is needed. For a structure this characterisation by a single high-resolution image is less demanding than multiple experimental series to derive the parameter as in conventional procedures. In addition, the transport properties of very thin layers, of materials that are difficult to study in the Wicke-Kallenbach cell, or of virtually designed materials for which structural information is available from simulations but no physical sample has yet been synthesized, can be determined. The presented approach can be applied to any porous material permeated by a gas (or multiple gases), e.g. membranes, filters in general, bulk material, column internals, etc.

The method applied here is asymptotic homogenization, which allows structural information on the micro scale to be lumped into effective transport properties. The key idea of asymptotic homogenization is based on expressing the real physical problem as a representative mathematical problem (the so-called cell problem). The solution of the cell problem is directly related to the effective transport properties on a macroscopic scale. By variation of characteristic geometric properties of a porous structure, various kinds of pore structures can be covered. The resulting basic functions are integrated to calculate the effective transport properties of the up-scaled model. We applied this approach to porous media to derive the dusty-gas model parameters, namely permeability, Knudsen-diffusion and binary diffusion coefficient. In our present work, as well as in our previous work [2], we compare the model predictions based on cross sectional images with experimental data and literature data to validate our results. A remarkable agreement between experiment and simulation is achieved.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

[1] E. Wicke and R. Kallenbach, "Die Oberflächendiffusion von Kohlendioxyd in aktiven Kohlen," *Kolloid-Zeitschrift*, vol. 97, no. 2, pp. 135–151, Nov. 1941, doi: 10.1007/BF01502640.

[2] J. H. Matthies et al., "Up-scaling transport in porous polymer membranes using asymptotic homogenization," *Int. J. Numer. Methods Heat Fluid Flow*, Nov. 2019, doi: 10.1108/HFF-04-2019-0326. **Acceptance of Terms and Conditions:**

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MS8 / 745

## **Effective dispersion coefficients for the upscaling of pore-scale mixing and reaction in heterogeneous porous media**

**Authors:** Alexandre Puyguiraud<sup>1</sup> ; Lazaro Perez<sup>2</sup> ; Juan J. Hidalgo<sup>3</sup> ; Marco Dentz<sup>3</sup>

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We upscale reactive mixing using effective dispersion coefficients to capture the combined effect of pore-scale heterogeneity and molecular diffusion on the evolution of the mixing interface between two initially segregated dissolved species. These effective dispersion coefficients are defined as the average spatial variance of the solute plume that evolves from a pointlike injection (the transport Green function).

We numerically investigate the effective longitudinal dispersion coefficients in two porous media of different structure heterogeneity and through different Péclet number regimes for each medium. We find that, as distance traveled increases (or time spent), the solute experiences the pore-scale velocity field heterogeneity due to advection and transverse diffusion, resulting in an evolution of the dispersion coefficients. They evolve from the value of molecular diffusion at early time, then undergo an advection dominated regime, to finally reach the value of hydrodynamic dispersion at late times. Thus, at times smaller than the diffusion time over a characteristic pore length, the effective dispersion coefficients can be significantly smaller than the hydrodynamic dispersion coefficients. Therefore, mismatches between pore-scale reaction data from experiment or simulations and Darcy scale predictions based on temporally constant hydrodynamic dispersion can be explained through these differences. We use the effective dispersion coefficients to approximate the transport Green function and to quantify the incomplete mixing occurring at the pore-scale. We evaluate the evolution of two initially segregated species via this methodology. The dispersive lamella approach accurately predicts the evolution of the product mass of an instantaneous bimolecular reaction obtained from direct numerical simulations. These results shed some new light on pore-scale mixing, the notion of incomplete mixing, and its prediction and upscaling in terms of an effective mixing model.

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MS8 / 292

## **Effects of Inertia and Diffusion on Reactive Transport with Fluid-Solid Reactions in Rough Fractures**

**Author:** Woonghee Lee<sup>1</sup>

**Co-authors:** Seonkyoo Yoon<sup>1</sup> ; Peter Kang<sup>1</sup>

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Fluid-solid reactions in rough fractures govern many biogeochemical reactions that are relevant to various subsurface processes and applications, and fluid flow often exerts a dominant control over fluid-solid reactions. In particular, recirculating flows in rough fractures have been shown to induce anomalous transport, characterized as the nonlinear scaling of the second spatial moment of particles in time. Recirculating flows readily occur in fracture flows by the interplay between fluid inertia and rough walls, and the interplay between recirculating flows and molecular diffusion determine the trapping effects of recirculating flows. However, the effects of fluid inertia and molecular diffusion on reactive transport with fluid-solid reactions have not been comprehensively studied.

In this study, we investigate the effects of fluid inertia and solute diffusion on solute transport with fluid-solid reactions and propose an upscaled reactive transport model that effectively captures reactive transport. We simulate reactive transport with fluid-solid bimolecular reactions,  $A + \text{Solid} \rightarrow C$ , with a Lagrangian-based transport-reaction model. We assume an instantaneous irreversible reaction, where C particles are immediately generated when A particles collide with fracture surfaces. We explore a wide range of Reynolds (Re) and Peclet (Pe) numbers, and recirculating flows are shown to govern reactive transport by increasing the residence time of C particles through trapping effects and also facilitate the reaction by increasing the residence time of A particles near fracture walls. Recirculating flows also induce a preferential flow path that leads to enhanced spreading, which in turn affects fluid-solid reactions. Based on the improved understanding, we upscale reactive transport with velocity-dependent effective reaction rates. We compare upscaled models with velocity-dependent and velocity-independent reaction models and show that the velocity-dependent reaction model improves the predictability of the upscaled model.

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MS25 / 725

## Effects of Soil Heterogeneity and Transient Flow on Multicomponent Biodegradation

**Authors:** Darrell Tang<sup>1</sup> ; Sjoerd van der Zee<sup>1</sup>

<sup>1</sup> *Wageningen University*

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Aerobic biodegradation is an important mechanism of organic contaminant removal from soils. We simulate nonlinear multicomponent biodegradation and transport of contaminants in spatially auto-correlated heterogeneous unsaturated soils under transient infiltration conditions. These processes introduce spatio-temporally complex behaviour that affect contaminant travel times, the extent of reactant mixing, solute and biomass distributions in the soil, and thus also biodegradation and leaching outcomes. In heterogeneous soils, significant changes in infiltration rate may induce switching of preferential flow zones, as discussed by Roth (1995). Such interactions between the modelled complex processes also determine the extent of biodegradation. Behaviour is found that essentially differs from simplified models with monocomponent biodegradation, homogeneous soils, or steady flow. Under mixing-limited conditions, soil heterogeneity is likely to significantly increase biodegradation. Heterogeneity is less impactful under rate-limited conditions, and is neither more likely to increase or decrease biodegradation. Multicomponent biodegradation is more likely mixing-limited when infiltration rates are small, contaminant concentrations are high, and electron acceptors are abundant. Transient flow has little effect on rate-limited scenarios, but significantly decreases biodegradation in some mixing-limited scenarios. This decrease is more likely in homogeneous than in heterogeneous soils. Under transient flow, preferential flow zone switching reduces the spatiotemporal heterogeneity of biomass and contaminant concentrations, and contaminant plumes have a smaller upstream tail because there are less stagnant flow zones for contaminants to be trapped in. For the same reasons, transient flow also reduces outcome variability across heterogeneous realizations with identical macroscopic properties. Altogether, the results suggest that flow rate variability tends to suppress the effects of soil heterogeneity, while soil heterogeneity decreases the influence of flow rate variability. Furthermore, the influence of additional model complexity on outcomes is larger for mixing-limited than rate-limited biodegradation. Numerical models of multicomponent biodegradation may be simplified accordingly, allowing the computational burden of simulations to be reduced when necessary.



**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

Roth, K. (1995). Steady State Flow in an Unsaturated, Two-Dimensional, Macroscopically Homogeneous, Miller-Similar Medium. *Water Resources Research*, 31(9), 2127-2140. **Acceptance of Terms and Conditions:**

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Poster + / 73

## Effects of nanopore geometry on confined water flow: a view of lattice Boltzmann simulation

**Authors:** Wen Zhao<sup>None</sup> ; Lin Jiang<sup>1</sup> ; Chengzao Jia<sup>1</sup><sup>1</sup> *Research Institute of Petroleum Exploration and Development***Corresponding Authors:** dlzhaowen@163.com, zhaowencup@126.com, zhaow625@126.com

Water flow in nanoscale channel is known to be affected by the strong water-wall interactions which induces that the flow significantly deviates from the conventional continuum flow. Vast experimental observation and simulation results in recent literature shows higher/lower-than-expected flow capacity in nanopores. Currently, most research are limited on the simple geometry with circular cross section. However, the flow dynamics of water in noncircular pores deviates from the Hagen-Poiseuille flow equation used in circular pores with various contact angles and dimensions significantly. In this work, molecular interactions between water and the solid inner wall are incorporated into Lattice Boltzmann method formulations to simulate the flow dynamics in nanopore with different cross-sectional shapes and wettability. When cross-sectional area injection pressure is identical, the circular nanopore has the strongest flow capacity. For circular cross-sectional shape, the constant density lines are also circular and concentric. For angular cross-sectional shape, the constant density lines become inconsistent with cross-sectional shape, the density varies greatly at the corner. The effects of geometry and density distribution of different contact angles have been analyzed in details. An empirical formula has been established which is of great use value in engineering field.

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Poster + / 818

## Efficient Numerical Design of Porous Materials With Target Properties and Microstructure

**Authors:** Benjamin Paisley<sup>1</sup> ; M. Sadegh Riasi<sup>1</sup> ; Mircea Grigoriu<sup>2</sup> ; Lilit Yeghiazarian<sup>1</sup><sup>1</sup> *University of Cincinnati*<sup>2</sup> *Cornell University*

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Despite recent advances in synthesis and manufacturing of porous materials and devices, producing porous structures with targeted properties is still an expensive, trial-and-error procedure. A powerful way to accelerate this process and to guide manufacturing is to use numerical design of porous media. Current numerical porous media design methodologies typically include a random microstructure generator nested within an optimization routine. At each iteration, the optimization algorithm compares properties of the microstructure such as permeability, porosity, and pore size distribution with their desired target values and modifies the inputs to the generator accordingly. A considerable drawback of this approach is computational cost, which is mainly due to the time needed to generate a completely new microstructure and to compute the corresponding properties at each iteration. To address this problem, we propose the adjustable level-cut filtered Poisson field (ALCPF) method, a new approach based on the level-cut Poisson field theory. First, several initial domains are generated based on a set of filtered Poisson field parameters. Then, rather than generating a completely new field, the optimization algorithm takes a weighted geometric average of the initial domains to produce an updated random field. Material properties of the generated sample are then computed using a fast pore topology method (PTM). The weights are adjusted until an optimal domain is found. With up to threefold reduction in computational time, this method successfully matches target pore size distribution, pore size gradient and permeability at a wide range of porosities.

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**Poster + / 764**

## **Efficient methane gas production strategies from gas hydrate reservoir using the numerical simulations**

**Authors:** Neelam Choudhary<sup>None</sup> ; Jyoti Phirani<sup>1</sup>

<sup>1</sup> *IIT, Delhi*

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The numerical simulations of the gas hydrate reservoir are used to predict the reservoir response during the production tests. The complexity of the gas hydrate reservoir needs to be carefully studied through the reservoir simulations to model the long-term production tests. The feasibility of the gas production has already been demonstrated from the short-term production tests. However, the critical issues remain challenging during the long-term production. In the present work we analyze the efficient production method as well as the gas production behavior due to different well arrangements and the operating conditions. A 3-D oceanic class-2 reservoir block underlain by an unconfined aquifer layer is modeled in this work.

An In-house multiphase, multicomponent, thermal 3-D finite volume legacy simulator is used with 3 components- water, methane, and hydrate in four phases – gas, aqueous, hydrate and ice. Energy and mass balance equations are solved in space and time domain to compute the production of gas in a reservoir. The depressurization method in an unconfined reservoir becomes ineffective for the vertical wells as well as the horizontal wells. Therefore, warm water injector is used along with the depressurization to explore the impact of different arrangements of horizontal and vertical well. The horizontal wells are more efficient as compared to the vertical wells. The gas produced is 48% original gas in place (OGIP) for horizontal injectors compared to the 22% of OGIP for vertical injectors. The unconfined aquifer layer plays an important role in the gas production using different locations of the horizontal wells. When the horizontal injector is located near the aquifer layer, gas production starts from the day one as the aquifer layer makes water convection easier. However, when the injector is located in the low permeability hydrate layer, the gas production start only after the dissociation front reaches the aquifer, delaying the gas production for initial days. We also

investigate the impact of initial reservoir conditions on the gas production. The initial reservoir pressure determines the effectiveness of the depressurization method and have larger impact on the production as compared to the other initial reservoir conditions.

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MS21 / 228

## Elastic turbulence generates anomalous flow resistance in porous media

**Authors:** Christopher Browne<sup>1</sup> ; Sujit Datta<sup>2</sup>

<sup>1</sup> *Princeton University*

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Polymer solutions are often injected in porous media for applications such as oil recovery and groundwater remediation. In many cases, the macroscopic flow resistance abruptly increases above a threshold flow rate in a porous medium, but not in bulk solution. The reason why has been a puzzle for over half a century. Here, by directly visualizing the flow in a transparent 3D porous medium, we demonstrate that this anomalous increase is due to the onset of an elastic instability in which the flow exhibits strong spatio-temporal fluctuations reminiscent of inertial turbulence, despite the vanishingly small Reynolds number. We find that the transition to unstable flow in each pore is continuous, arising due to the increased persistence of discrete bursts of instability above an onset flow rate; however, this onset value varies from pore to pore. Thus, unstable flow is spatially heterogeneous across the different pores of the medium, with unstable and laminar regions coexisting. Guided by these findings, we quantitatively establish that the energy dissipated by unstable pore-scale fluctuations generates the anomalous increase in flow resistance through the entire medium. Thus, by linking the onset of unstable flow at the pore scale to transport at the macroscale, our work provides generally-applicable guidelines for predicting and controlling polymer solution flows.

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MS13 / 211

## Elasticity of argon in nanopores of different sizes

**Authors:** Klaus Schappert<sup>1</sup> ; Rolf Pelster<sup>1</sup>

<sup>1</sup> *Universität des Saarlandes*

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The elastic properties of porous media are of great relevance in many fields of research. Previous ultrasonic measurements indicate an enhancement of the elastic moduli of adsorbates in nanoconfinement and their dependence on the Laplace pressure [1]. Simulations by Gor et al. have shown that the adsorbate's elasticity is related to the solvation pressure, which also causes the deformation of a porous material during sorption [2]. Thus, for a fully saturated porous material the dependence of the solvation pressure on the pore radius should cause an inverse proportionality between modulus and pore size [2].

Here, we study the effective longitudinal modulus of argon in porous glass samples with different pore sizes and we discuss the effects of nanoconfinement on the adsorbate's elasticity. We have measured the transit times of longitudinal ultrasonic waves propagating through the samples as a function of the relative pressure  $p/p_0$  (with the saturation vapor pressure  $p_0$ ). From these measurements we determine the effective longitudinal modulus, and we show how changes in the modulus during filling are influenced by the pore size.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

[1] Klaus Schappert and Rolf Pelster, Elasticity and Phase Behavior of Fluids in Nanoporous Media, pp. 259-304 in *Soft Matter and Biomaterials on the Nanoscale*, vol. 1, Patrick Huber, Ed. (World Scientific, 2020)

[2] Gennady Y. Gor, Christopher D. Dobrzanski and Alina Emelianova, Thermodynamic Fingerprints of Nanoporous Materials on the Fluids Confined in Their Pores, pp. 227-258 in *Soft Matter and Biomaterials on the Nanoscale*, vol. 1, Patrick Huber, Ed. (World Scientific, 2020) **Acceptance of Terms and Conditions:**

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Poster + / 146

## Electrical Impedance Spectroscopy: a tool to investigate interactions between complex fluids – porous materials

**Authors:** Nicolae Tomozeiu<sup>1</sup> ; Helder Salvador<sup>1</sup>

<sup>1</sup> Canon Production Printing

**Corresponding Authors:** nicolae.tomozeiu@cpp.canon, helder.marquessalvador@cpp.canon

An overview of the Electrical Impedance Spectroscopy (EIS) method targeting the physical processes specific to the water-based ink/substrate interaction is made in this work. After a brief introduction of the EIS technique, two experimental setups will be presented as the main EIS measurement instruments: planar and respectively cylindrical electrodes. They have been employed to study material properties (e.g. dielectric constants) of complex materials as well as physical phenomena as water evaporation of aqueous mixtures, complex liquid transport into porous paper, latex film formation. Each experimental setup was dedicated to a specific process; regarding the dielectric constant measurements, this was possible to be made with both setups and a comparison of the outputs is made.

EIS was used for:

- i) water evaporation from liquid mixtures;
- ii) liquid penetration into porous paper considering the same liquid and different papers (e.g. thickness), as well the same paper and various liquids;
- iii) latex film formation – revealing the structure of the solid formed film, have been tackled via the EIS method.

The dynamics of the physical processes (e.g. evaporation rate, liquid absorption rate, phases in latex film formation) have been studied having time as a parameter. Theoretical models and computational

simulations were used to analyze the experimental data and to improve our understanding. We consider the EIS as a valuable tool in these studies; however besides its advantages, we will discuss the limitations of the method, too.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

E. Barsoukov, and J. R. Macdonald, Impedance Spectroscopy: Theory, Experiment, and Applications, 2nd Edn., John Wiley & Sons, 2005  
M. Grossi and B. Riccò, *J. Sens. Sens. Syst.*, 6, 303–325, 2017  
N. Tomozeiu, *Transport in Porous Media*, Vol.115, No.3, 603-629, 2016 **Acceptance of Terms and Conditions:**

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Poster + / 323

## Electrokinetic delivery of reactants in porous media: solution chemistry controls transport, mixing and degradation

**Authors:** Riccardo Sprocati<sup>1</sup> ; Andrea Gallo<sup>2</sup> ; Rajandrea Sethi<sup>2</sup> ; Massimo Rolle<sup>1</sup>

<sup>1</sup> *Technical University of Denmark*

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Electrokinetic phenomena occur in porous media as a result of the application of electric potential gradients. This technique has great potential for remediation of soil and groundwater even in challenging low-permeability porous media. The applied, low-intensity electric fields can enhance the transport of contaminants and the delivery of reactants and amendments for in situ (bio)degradation. In this work we focus on electromigration, typically the most important mechanism of electrokinetic transport in subsurface porous media, and we experimentally demonstrate that changes in chemical conditions such as the concentration of a background electrolyte in the pore water of a saturated porous medium, control the macroscopic transport of charged tracers and reactants [1]. In a first set of experiments, we demonstrate that during electrokinetics the differences between the concentration of a tracer electrolyte and a background solution can significantly influence the delivery of the injected tracer, its spatial distribution and its mixing behavior with respect to a comparable scenario of advective-dispersive transport. In a second set of experiments, we show the implications of such electrokinetically-induced charge interactions for a reactive system, considering chemical oxidation of a non-charged organic compound (glucose) by a charged reactant (permanganate). The experimental results are quantitatively interpreted with numerical simulations, performed with the multiphysics and multicomponent model NP-Phreeqc-EK [2]. The outcomes of this study open interesting perspectives on electrokinetic approaches to design and implement effective delivery and remediation strategies in subsurface porous media [3].

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

[1] Sprocati, R., Gallo, A., Sethi, R., & Rolle, M. (2021). Electrokinetic Delivery of Reactants: Pore Water Chemistry Controls Transport, Mixing, and Degradation. *Environmental Science & Technology*, 55 (1), 719–729.

[2] Sprocati, R., Masi, M., Muniruzzaman, M., & Rolle, M. (2019). Modeling electrokinetic transport and biogeochemical reactions in porous media: A multidimensional Nernst–Planck–Poisson approach with PHREEQC coupling. *Advances in Water Resources*, 127, 134-147.

[3] Sprocati, R., Flyvbjerg, J., Tuxen, N., & Rolle, M. (2020). Process-based modeling of electrokinetic-enhanced bioremediation of chlorinated ethenes. *Journal of Hazardous Materials*, 397, 122787. **Acceptance of Terms and Conditions:**

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**MS6-A / 447**

## Energy dissipated through Haines jumps in disordered media

**Authors:** Ran Holtzman<sup>1</sup> ; Marco Dentz<sup>2</sup> ; Ramon Planet<sup>3</sup> ; Jordi Ortin<sup>3</sup>

<sup>1</sup> *Coventry University*

<sup>2</sup> *IDAEA-CSIC*

<sup>3</sup> *Universitat de Barcelona*

**Corresponding Authors:** rholtzman4@gmail.com, jordi.ortin@ub.edu, ramon.planet@gmail.com, marco.dentz@csic.es

We study energy dissipation in quasistatic two-fluid displacements in disordered media, analytically, numerically and experimentally. We establish the energy balance for a recent model that successfully reproduces collective capillary instabilities (Haines jumps), hysteresis and memory of pressure-saturation trajectories [1]. Strikingly, we discover that energy dissipation can emerge from cooperative behavior mediated by lateral correlations between individually reversible capillary displacements. This contrasts the widely-used compartment (Everett) model which rely on the existence of a basic noninteracting hysteretic unit.

We find that the energy dissipated in individual Haines jumps between two consecutive equilibrium configurations (i) needs not to be proportional to the corresponding increase in saturation (avalanche size), (ii) spans many orders of magnitude, and (iii) can greatly exceed the work invested in driving the system between these two configurations. We study parametrically how the dissipation depends on system properties such as the microstructural heterogeneity and gravity (Bond number). Finally, we expose the connection between dissipation and large-scale imbibition-drainage hysteresis. We show that the accumulated dissipation along a cyclic pressure-saturation trajectory coincides with the area enclosed by the cycle.

[1] Holtzman, R. et al., Nature Communications Physics, 3:222 (2020).

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10.1038/s42005-020-00492-1 **Acceptance of Terms and Conditions:**

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**MS6-A / 8**

## Energy dissipation as heat in porous media flow

**Authors:** Signe Kjelstrup<sup>1</sup> ; Dick Bedeaux<sup>2</sup> ; Olav Galteland<sup>1</sup> ; Michael Rauter<sup>1</sup> ; Carl Fredrik Berg<sup>1</sup> ; Alex Hansen<sup>1</sup>

<sup>1</sup> *Norwegian University of Science and Technology*

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The most common way to describe two-phase flow in porous media is to use the relative permeability equations for each phase. Also non-linear flux-force relations are now documented and in use. The energy dissipation can in both cases be well described by the entropy production in the system, or alternatively by the net entropy flow out of the system at steady state. Some of us have proposed to define the number of state variables in REV in a way that reduces the number of variables considerably [1]. The concept of local equilibrium in the REV has been explained and used to build an expression for the entropy production.

As the entropy production is invariant at any scale, we can use it to examine different sets of variables. A set of constitutive equations will follow, for which the Onsager relations should hold. First evidence in this direction has been found [2]. We explain how transport equations can be defined from on basis, in particular how the thermodynamic driving forces can be defined. We illustrate definitions by numerical and molecular simulations.

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[1] Signe Kjelstrup, Dick Bedeaux, Alex Hansen, Bjørn Hafskjold, Olav Galteland, Non-isothermal transport of multi-phase fluids in porous media. The entropy production. *Frontiers in Physics* 6 (2018) 126 doi: 10.3389/fphy.2018.00126

[2] Mathias Winkler, Magnus Aa. Gjennestad, Dick Bedeaux, Signe Kjelstrup, Rafaela Cabriolu, Alex Hansen, Onsager-Symmetry Obeyed in Athermal Mesoscopic Systems: Two-Phase Flow in Porous Media, *Frontiers in Physics* 8 (2020) 60 doi: 10.3389/fphy.2020.00060 **Acceptance of Terms and Conditions:**

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MS5 / 190

## Enzymatic degradation of biomass: a porous media approach

**Authors:** Sarah Blossé<sup>1</sup> ; Antoine Bouchoux<sup>2</sup> ; Paul Duru<sup>3</sup> ; Cédric Montanier<sup>2</sup>

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<sup>2</sup> *Toulouse Biotechnology Institute, Université de Toulouse, CNRS, INRA, INSA - Toulouse, France*

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In the present era marked by the desire to build a bio-economy, plant biomass has a vast potential as a source of renewable and environmentally friendly molecules of interest. Deconstruction of biomass by a cocktail of enzymes is relevant at an industrial scale. However, achieving a better understanding of the intimate relationship between synergistic enzymatic activity and deconstruction of mechanisms of enzymatic degradation of such a complex, multiscale porous material is still needed.

In this work, we present some results regarding enzymatic degradation of a model biomass, raw wheat straw, obtained with experimental approaches such as X-Ray tomography or breakthrough curve analysis, which are usually dedicated to more “conventional” porous media.

First, we will present some results obtained using a laboratory-scale X-ray tomograph. Fully hydrated wheat straw samples, placed in a home-made 3D-printed thermostatically controlled bioreactor, are subjected to action of a commercial enzymatic cocktail. Enzymatic activity is monitored using state of the art techniques in enzymology. In spite of a rather limited spatial resolution (voxel size is 1.25  $\mu\text{m}$ ), 3D X-ray tomography allows to highlight the selective effects of the enzymatic degradation. Notably, the disappearance of cellulose-rich cell walls as a function of the duration of

the enzymatic attack, can be quantified over the full scale of the wheat straw sample (i.e. a few mm in length) offering 3D pieces of information on the degradation process, which contrasts with the 2D picture classically obtained from 2D imaging techniques.

Second, in order to probe the effects of the enzymatic degradation at a sub-micron scale, we analyse breakthrough curves obtained by 2D X-ray radiography, when flushing with pure water a wheat straw initially saturated with a radio-opaque molecular tracer. Experiments are conducted with untreated and degraded wheat straws. Breakthrough curve analysis is used to detect any differences between these two kinds of samples, which traduce an alteration of the transport properties of the tracer within the wheat straw. Modelling of the transport properties (e.g. through an effective diffusion coefficient) in relation with the enzymatic degradation mechanism (e.g. progressive disentangling of the polymer network constitutive of the plant cell walls, prior to its disappearance as imaged on 3D images) is a key point and preliminary results will be presented.

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**Poster + / 509**

## **Estimation of auto-covariance of log hydraulic conductivity from Generalized sub-Gaussian porosity and particle size random fields**

**Author:** Matthew Harrison<sup>1</sup>

**Co-authors:** Mohaddeseh Mousavi Nezhad<sup>2</sup> ; Monica Riva<sup>3</sup> ; Alberto Guadagnini<sup>3</sup>

<sup>1</sup> *University of Warwick*

<sup>2</sup> *Associate Professor*

<sup>3</sup> *Politecnico di Milano*

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Several techniques which are widely employed for the estimation of hydraulic parameters of aquifer systems are based on particle-size and porosity information. These rely on empirical formulations which are usually adopted to obtain hydraulic conductivity from quantiles of particle size curves and porosity. We present analytical formulations relating the spatial covariance of the (natural) logarithm of hydraulic conductivity and that of representative soil particle sizes and porosity, as embedded in the classical Terzaghi model. Our exact formulations are then approximated through perturbation methods to yield workable expressions embedding the relationship between the main geostatistical descriptors of sedimentological and hydraulic parameters of heterogeneous aquifer systems. We rest on a stochastic framework of analysis viewing a transformation of characteristic particle size ( $d_{10}$ ) and porosity as Generalized sub-Gaussian (GSG) spatially (cross-)correlated random processes. Typical low order statistics for  $d_{10}$  are determined for coarse sand using a global dataset of more than 400 unlithified samples from four different depositional environments. The accuracy of the resulting second-order (in terms of variance of porosity and characteristic particle diameter) model is assessed through a detailed suite of numerical Monte-Carlo analyses for typical values of estimated variance of porosity and  $d_{10}$ . We find that our low order analytical approximation of log-conductivity covariance is characterized by a remarkable agreement against its Monte Carlo based counterpart also for highly heterogeneous settings considering either cross-correlated or independent transformed porosity and  $d_{10}$  bivariate distributions.

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MS25 / 647

## Estimation of unsaturated soil hydraulic properties by integrated hydrogeophysical inversion of time-lapse ground-penetrating radar measurements

**Authors:** Khan Zaib Jadoon<sup>1</sup> ; Lutz Weihermüller<sup>2</sup> ; Sebastian Lambot<sup>3</sup> ; Davood Moghadas<sup>4</sup> ; Harry Vereecken<sup>2</sup>

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Ground-penetrating radar (GPR) has shown a great potential for high resolution and non-invasive mapping to estimate soil hydraulic parameters at the field scale. In traditional GPR methods, soil dielectric permittivity is retrieved by using ray-based travel time or reflection analyses, which is strongly correlated to soil moisture. These methods suffer, however, from two major shortcomings. First, only a part of the information in the GPR signal is considered (e.g., propagation time). Second, the forward model describing the radar data is subject to relatively strong simplifications with respect to electromagnetic wave propagation phenomena. These limitations typically results in errors in the reconstructed water content images and, furthermore, this does not permit to exploit all information contained in the GPR data.

We explored an alternative method by using full-waveform hydrogeophysical inversion of time-lapse off-ground GPR measurements to remotely estimate the unsaturated soil hydraulic properties. The radar system is based on international standard vector network analyzer technology and a full-waveform model is used to describe wave propagation in the antenna-air-soil system, including antenna-soil interactions. A hydrodynamic model is used to constrain the inverse electromagnetic problem in reconstructing continuous vertical water content profiles. In that case the estimated parameters reduce to the soil hydraulic properties, thereby strongly reducing the dimensionality of the inverse problem.

We present an application of the proposed method to a data set collected in lab and field experiments. The GPR model involves a full-waveform frequency-domain solution of Maxwell's equations for wave propagation in three-dimensional multilayered media. The hydrodynamic model used in this work is based on a one-dimensional solution of Richards equation and the hydrological simulator HYDRUS 1-D was used with a single- and dual-porosity model. To monitor the soil water content dynamics, time-lapse GPR and time domain reflectometry (TDR) measurements were performed, whereby only GPR data was used in the inversion. Significant effects of water dynamics were observed in the time-lapse GPR data and in particular precipitation and evaporation events were clearly visible. The dual porosity model provided better results compared to the single porosity model for describing the soil water dynamics, which is supported by field observations of macropores. Furthermore, the GPR derived water content profiles reconstructed from the integrated hydrogeophysical inversion were in good agreement with TDR observations. These results suggest that the proposed method is promising for non-invasive characterization of the shallow subsurface hydraulic properties and monitoring water dynamics at the field scale.

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MS5 / 547

## Evaluating the interaction of biofilms, organic matter and soil structures at the pore scale

**Author:** Alexander Prechtel<sup>1</sup>

**Co-authors:** Simon Zech<sup>2</sup>; Alice Lieu<sup>3</sup>; Raphael Schulz<sup>4</sup>; Nadja Ray<sup>5</sup>

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Key functions of soils, such as permeability or habitat for microorganisms, are determined by structures at the microaggregate scale ( $< 250 \mu\text{m}$ ).

Although advanced imaging techniques now allow snapshots even down to the nanoscale, the evolution of elemental distributions and dynamic processes still can often not be assessed experimentally. So mechanistic models operating at the pore scale can help to study and understand such phenomena.

We consider the complex coupling of biological, chemical, and physical processes in a hybrid discrete-continuum modeling approach. It integrates dynamic wetting (liquid) and non-wetting (gas) phases including biofilms, diffusive processes for solutes, mobile bacteria transforming into immobile biomass, and ions which are prescribed by means of partial differential equations. Furthermore the growth of biofilms as, e.g., mucilage exuded by roots, or the distribution of particulate organic matter in the system, is incorporated in a cellular automaton framework (CAM) presented in [1, 2, 3]. It also allows for structural changes of the porous medium itself (see, e.g. [4]). As the evolving computational domain leads to discrete discontinuities, we apply the local discontinuous Galerkin (LDG) method for the transport part.

Finally mathematical upscaling techniques are used to incorporate the information from the pore scale to the macroscale [1,5].

The model is applied for two research questions: Although a continuous re-organization of disintegrating and assembling soil aggregates can be observed, we still lack understanding of the mechanistic relationship between aggregation and organic matter sequestration in soils. We model the incorporation and turnover of particulate OM influencing soil aggregation. We hypothesize that soil mineral surfaces co-located with decomposing OM develop into spatially discrete ‘gluing’ hotspots that enhance aggregation locally and tested different numerical scenarios of OM input regimes, OM turnover, particle size distribution and ‘gluing’ hotspots.

As a second application, we quantify the effective diffusivity by upscaling on 3D geometries from CT scans of a loamy and a sandy soil. We see that conventional models for diffusivity cannot account for natural pore geometries and varying phase properties. Upscaling allows also to quantify how root exudates (mucilage) can significantly alter the macroscopic soil hydraulic properties.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

- [1] N. Ray, A. Rupp and A. Prechtel. Discrete-continuum multiscale model for transport, biomass development and solid restructuring in porous media. *Advances in Water Resources*, 107, 393-404, (2017).
- [2] A. Rupp, K. Totsche, A. Prechtel and N. Ray. Discrete-continuum multiphase model for structure formation in soils including electrostatic effects. *Frontiers in Environmental Science*, 6, 96, (2018).
- [3] Y. Tang and A.J. Valocchi. An improved cellular automaton method to model multispecies biofilms. *Water Research*, 47(15), 5729-5742, (2013).

[4] S. Zech, S. Dultz, G. Guggenberger, A. Prechtel and N. Ray. Microaggregation of goethite and illite evaluated by mechanistic modeling. *Applied Clay Science* 198, 105845 (2020).

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**Poster + / 297**

## Evaluation of mineral surface area evolution during dissolution reactions

**Author:** Fanqi Qin<sup>None</sup>

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Geochemical reactions in porous media can result in various patterns of flow channels and fractures which could potentially alter the properties of the porous media including porosity, permeability, tensile strength and tortuosity, etc. Enhancing our knowledge of these reactions at pore scale can help better predict the impacts of these reactions on the larger scales. Mineral surface area, as one of the controlling parameters in geochemical reactions, can be measured or estimated in various methods such as geometry, BET adsorption, imaging, etc. It has been reported in the literature that the estimated mineral surface area can vary up to 5 orders of magnitude. In addition, the knowledge on how mineral surface area evolves during the geochemical reactions is lacking. Currently, the commonly used theory assumes that mineral grains to be a smooth sphere and the surface area changes with changing sphere size. However, backscatter electron (BSE) images of rock samples revealed that most of the mineral grains are not spherical, and has different level of surface roughness. In this work, the evolution of mineral surface area will be evaluated for different mineral phases through core-flood experiments. Hydrochloric acid (HCl) will be used as the reacting fluid in the core-flood experiment with a half-inch core (Bandera Grey). Inductively coupled plasma-optical emission spectrometry (ICP-OES) will be used to determine the effluent chemistry, from which the reaction rate and reactive surface area can be estimated. Scanning electron microscopy (SEM) backscatter electron (BSE) images will be used to estimate mineral accessible surface areas and to compare the surface change of different mineral phases before and after experiments. X-ray micro computed tomography (micro-CT) will be used to analyze the pore space change and newly formed flow channels. Based on the experimental data and observations, we aim to find a relationship among porosity, volume fraction and mineral surface areas.

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**MS19 / 460**

## Evaluation of the Impact of Flow Field Design on the Porosity of

## Zinc Deposition in the Zinc-Iodide Flow Battery by X-ray Computed Tomography

**Authors:** Fatemeh ShakeriHosseinabad<sup>1</sup> ; Sohrab Randjbar Daemi<sup>2</sup> ; Paul Shearing<sup>3</sup> ; Edward (Ted) P.L.Roberts<sup>4</sup>

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Among the aqueous redox flow battery systems, redox chemistries using a zinc negative electrode have a relatively high energy density [1]. In this study, a new flow field design was applied in a zinc-iodide flow battery, with some of the electrolyte flowing over the electrode surface, and a fraction of the flow passing through the porous felt electrode in the direction of current flow. The flow battery was tested under constant current density and the efficiency, discharge energy density and power density of the battery were improved compared to conventional flow field designs. The morphology of the zinc deposition was studied using scanning electron microscopy and optical profilometry. It was found that the flow through the electrode led to a thinner zinc deposit with lower roughness on the surface of the electrode, in comparison to the case where there was no flow through the electrode.

During the charging process, metallic zinc is electroplated on the porous graphite felt in the negative side of the battery [2]. Ex-situ tomographic measurements were used to image the zinc particles on the surface and inside the porous felt qualitatively and quantitatively. Information of porosity, thickness and distribution of the zinc in the porous felt were obtained from x-ray computed tomography (XCT) images. Volume rendering of graphite felt from XCT images showed that in the presence of flow through the electrode, more zinc deposition occurred inside the porous felt, resulting in a thinner surface deposit, and higher battery capacity and improved performance.

[1]- Khor, A., P. Leung, M. R. Mohamed, C. Flox, Q. Xu, Liang An, R. G. A. Wills, J. R. Morante, and A. A. Shah. "Review of zinc-based hybrid flow batteries: From fundamentals to applications." *Materials today energy* 8 (2018): 80-108.

[2]- Li, Bin, Zimin Nie, M. Vijayakumar, Guosheng Li, Jun Liu, Vincent Sprenkle, and Wei Wang. "Ambipolar zinc-polyiodide electrolyte for a high-energy density aqueous redox flow battery." *Nature communications* 6, no. 1 (2015): 1-8.

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## Event-based measurements of contact angles during imbibition to evaluate contact angle hysteresis on a pore-by-pore basis using micro-CT

**Author:** Sharon Ellman<sup>1</sup>

**Co-authors:** Arjen Mascini<sup>2</sup> ; Tom Bultreys<sup>1</sup>

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Multiphase flow in porous rocks plays a key role in CO<sub>2</sub> sequestration, groundwater remediation and petroleum reservoir management. In the subsurface, drainage and imbibition typically take place at low capillary numbers, meaning capillary forces dominate the pore scale behavior. The fluid displacement is then strongly influenced by the wetting properties of the pore walls, which is typically characterized by defining an effective contact angle. Significant effort has been devoted to measuring contact angles in-situ on X-ray micro-computed tomography images of fluids in the pore space (AlRatrou et al., 2017; Sun et al., 2020). To maximize the relevance of the measured values to fluid displacement, Mascini et al. (2020) introduced an event-based approach, measuring local contact angles on time-resolved micro-CT data just before fluid redistribution events (Haines jumps) during drainage. Here, we assess whether event-based contact angles can be reliably determined during imbibition, considering the latter as a sequence of piston-like displacements, snap-offs and cooperative pore filling events. This can be compared with drainage measurements in order to evaluate contact angle hysteresis on a pore-by-pore basis. A contact angle analysis was performed on a glass beads dataset which consists of time resolved images taken during an imbibition experiment, using micro-computed tomography (Schlüter et al., 2016). The contact angles at every point on the three-phase-contact-line were determined for every time step. These were then used to identify imbibition events and calculate the event-based contact angles. Preliminary results reveal an average 8 degree contact angle hysteresis in individual pores for this dataset. Imbibition measurements reveal a positive correlation between event-based contact angles and time, while this relationship is not seen during drainage. The results indicate the existence of contact angle hysteresis, even in a medium as simple as a glass bead pack. Understanding and quantifying this hysteresis in the more complex media of porous rocks is crucial to understanding multiphase flow in nature.

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MS1 / 643

## Evolution of Bentheimer Sandstone Wettability During Cyclic scCO<sub>2</sub>-Brine Injections

**Author:** Anna Herring<sup>1</sup>

**Co-authors:** Zhe Li <sup>2</sup> ; Chenhao Sun <sup>3</sup> ; Ryan Armstrong ; James McClure <sup>4</sup> ; Mohammad Saadatfar <sup>5</sup>

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Geologic sequestration in sedimentary formations has been identified as a potential technology to prevent climate-change inducing carbon dioxide (CO<sub>2</sub>) from being emitted to the atmosphere. In order to achieve safe and effective storage underground, accurate understanding and predictions of CO<sub>2</sub> behavior in subsurface rock formations is required; including quantifying how much CO<sub>2</sub> is trapped within pore spaces by capillarity (vs. how much remains mobile), and constraining the occurrence of physio-chemical reactions between CO<sub>2</sub> and the mineral matrix. Experiments where

multiple cycles of CO<sub>2</sub> and brine are injected into rock samples have produced conflicting results; likely due to differences in mineral content of samples, pressure-temperature conditions, the suite of aqueous chemistry parameters which may impact results, and experimental apparatus and protocol. We present a new set of experiments, designed to replicate the conditions of a previous study, but with a new experimental design, apparatus, and timeline. We confirm the previous results that demonstrated shifts in CO<sub>2</sub> trapping behaviour over multiple injection cycles, and we conduct additional analyses to discern the fluid-fluid macroscopic contact angle, curvature, interfacial area, and topology of trapped CO<sub>2</sub> ganglia. The results are considered in the context of two mechanisms that could cause evolution of CO<sub>2</sub> behavior; (1) mineral fines migration, and (2) solubility-induced CO<sub>2</sub> adhesion and wettability alteration. We do not observe significant evidence of fines migration in this “clean” Bentheimer sandstone system. Conversely, Lattice-Boltzmann simulations based on the proposed conceptual model of wettability alteration exhibit similar trends in pressure measurements, end-point saturation levels, and CO<sub>2</sub> ganglia morphological characteristics as experiments, indicating that the changes observed in experiments could be due to wettability alteration as proposed. We observe that this wettability alteration renders CO<sub>2</sub> more stable in the rock pore space, increasing capillary trapping over four injection cycles.

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MS3 / 77

## Evolution of fracture permeability induced by THMC-coupled processes

**Author:** Xiangzhao Kong<sup>1</sup>

**Co-authors:** Marina Grimm Lima<sup>1</sup> ; Xintong Wang<sup>1</sup> ; Jin Ma<sup>2</sup>

<sup>1</sup> *Geothermal Energy and Geofluids (GEG) Group, Department of Earth Sciences, ETH Zurich*

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Coupled thermal-hydrological-mechanical-chemical (THMC) processes can significantly impact fracture permeability, immediately influencing the productivity/injectivity of fracture-dominated reservoirs, associated with geothermal energy extraction, hydrocarbon production, nuclear waste disposal, and geologic storage of carbon dioxide (CO<sub>2</sub>). It is, therefore, necessary to investigate the THMC coupling processes in natural fractures to develop well-calibrated models and predict the changes in hydraulic and transport properties of deep geological reservoirs.

In this presentation, results of flow-through experiments on fracture granite samples were reported to examine permeability evolution induced by THMC-coupled processes. We used two types of granite samples, naturally fractured granodiorite cores from the Deep Underground Geothermal Lab at the Grimsel Test Site (GTS) in Switzerland, and hydrothermally-altered fractured granite from Borehole EPS1 of the Soultz geothermal system and power plant site in France.

The GTS granite samples were subjected to flow-through experiments using DI water at temperatures varying 25-140 °C to characterize the evolution of fracture permeability. Periodic measurements of the efflux of dissolved minerals yield the net removal mass, which is correlated to the observed rates of fracture closure. Changes measured in hydraulic aperture are significant, exhibiting reductions of 20-75 % over the heating/cooling cycles.

The Soultz granite sample was first opened along the calcite-filled fracture, and then subjected to flow-through experiments using HCl solution at a temperature of 100 °C to evaluate the the evolution of fracture permeability and the fracture shear displacements due to calcite dissolution. Periodic

fluid samples were also taken to infer the efflux of dissolved minerals. A strong correlation can be observed between permeability and shear displacement of the fracture.

Our experimental observations in this study should certainly contribute to the interpretations on coupled THMC evolutions during processes such as chemical/thermal stimulation of enhanced geothermal systems and carbon capture, utilization, and storage.

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Lima, M.G., Vogler, D., Querci, L. et al. Thermally driven fracture aperture variation in naturally fractured granites. *Geotherm Energy* 7, 23 (2019). **Acceptance of Terms and Conditions:**

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MS13 / 387

## Examining the Structure of Supercritical CO<sub>2</sub> using X-ray Raman Spectroscopy and Atomistic Scale Modeling

**Author:** Priyanka Muhunthan<sup>None</sup>

**Co-authors:** Dimosthenis Sokaras<sup>1</sup> ; Matthias Ihme<sup>2</sup>

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Carbon capture and sequestration (CCS) involves the injection of supercritical carbon dioxide into tight rock formations such as shale. Previous studies have shown that such nanoconfinement leads to changes in phase behavior, including reduction in critical point and changes in interfacial surface tension. In this work, X-ray Raman Spectroscopy (XRS) is used to examine the structural changes of supercritical CO<sub>2</sub> during phase-transition. We combine XRS measurements, molecular dynamics simulations, and first principles density functional theory (DFT) calculations to characterize the local electronic structure of CO<sub>2</sub> near the critical point and crossing the Widom line. We observe clear differences in the spectral fingerprint of the oxygen K-edge spectra of liquid CO<sub>2</sub>, which is supported by DFT-based calculations. To understand the behavior of nanoconfined supercritical CO<sub>2</sub>, these experimental measurements are complemented by molecular-dynamics simulation to explain the observations and examine the molecular structure during the phase-transition.

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## Experimental Determination of Intrinsic In-Plane Permeability for Thin Porous Media

**Authors:** Luwen Zhuang<sup>1</sup> ; S. Majid Hassanizadeh<sup>2</sup>

<sup>1</sup> Sun Yat-sen University

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Nowadays, thin porous media have attracted much attention because of their importance to various industries. Hygiene products, paper, filters, fuel cells, membranes, textiles, muscular tissues, and other biological or manufactured thin compositions are widely encountered in daily life. The typical characteristic of a thin porous layer is that its thickness is much smaller than its in-plane dimensions. Determining the hydraulic properties is essential to understand and model fluid flow in thin porous media. In this presentation, we describe a new simple custom-built apparatus for measuring intrinsic permeability of a thin fibrous sheet in in-plane direction. Either water or gas can be injected into the setup as the fluid phase. We measured the permeability values for two types of thin fibrous porous media using either water or gas phase. The fibrous sheets were cut by 0 degree, 45 degrees, or 90 degrees to the fibers' direction. The results have shown that the measured values using gas phase were slightly larger than the ones obtained using water phase. The largest permeability value was found when the flow direction was paralleled to the fibers' direction.

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**Poster + / 280**

## Experimental Evaluation of Polymeric Fluid Displacement in Carbonates using an X-ray Imaging Technique

**Author:** Nara Brandão Costa Santos<sup>1</sup>

**Co-authors:** Arsalan Zolfaghari<sup>2</sup>; João Jorge Ribeiro Damasceno<sup>1</sup>; Fábio Oliveira Arouca<sup>1</sup>; Shahin Negahban<sup>3</sup>; Amir Masoud Kalantari Dahaghi<sup>3</sup>

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The filter cake formation during overbalanced drilling, and later on, its displacement and rearrangement during production are key parameters that impact formation damage, fluid loss control, and ultimately, effective production of hydrocarbon fluids. To address these issues, we investigate the impacts of non-Newtonian fluid rheology and pore space topology on the inner filter cake formation and its subsequent rearrangements as the result of a series of oil injections. We have performed two sets of experiments with two different concentrations of xanthan gum (XG) solutions (i.e., 0.2 and 0.4% w/w), and three different oil flow rates. The different oil flow rates mimic different areas of the reservoir during oil production. The cores were obtained from a water-wet carbonate outcrop and placed in aluminum core holders. One of the cores has a vertical fracture, the impact of which in terms of the XG-to-oil displacement is evaluated. We use the non-destructive 3D technique of X-ray micro-computed tomography (micro-CT) that enables tracking of pore fluid occupancy and visualizing the internal structures of the porous media. We have carried out extensive image analysis and proposed a novel methodology to account for the microporosity contribution to the total core porosity. Micropores are small pores that can not be identified at the acquired micro-CT resolution and are often seen as grey colors in the images. Reference and target-state images are taken after polymer injection and after each oil flooding, respectively. We first filtered the reconstructed images, then registered target and reference state images, and lastly segmented the XG and oil phases



from the resolved pore space. The final segmented images are analyzed to obtain saturation profiles, pores' attributes that hold a specific phase, and cluster size distributions. As the different cycles of oil injection were performed, the number of pores holding XG in the center decreased, and the polymer was left at small pores. The fracture is filled with oil right after the first drainage. We also identify polymer retention near the inlet face of both cores. In core 1 with a higher permeability value, the well-connected pore space favored the formation of large oil clusters and coalescence among the remaining XG clusters. In core 2 with less permeability, the thin throats and small pores hindered polymer displacement; thus, a higher residual XG saturation is achieved at the end of oil injection processes. Our experimental findings highlight the interplay of the reservoir's petrophysical characteristics and mud rheology in the filter cake formation and displacement behavior, giving an approach to reduce permanent damage and assess efficient oil production.

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## Experimental Investigation of Capillary Number's Control on Stress-Dependent Shifts in Irreducible Saturation in Deformable Porous Media

**Author:** Amir Haghi<sup>1</sup>

**Co-author:** Richard Chalaturnyk<sup>1</sup>

<sup>1</sup> *University of Alberta*

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Characterization of irreducible saturation of the wetting phase during multiphase fluid flow in porous media is essential for an accurate estimation of CO<sub>2</sub> storage capacity and hydrocarbon recovery of the geological formations. Despite pore deformation has been shown to significantly control single-phase and multiphase fluid flow in porous media, the interactive controls of capillary number and mechanical pore deformation on irreducible saturation during multiphase fluid flow in geo-materials is not yet fully explored. In this study, the stress-dependent shifts of irreducible water saturation (*Sw<sub>ir</sub>*) of a Berea sandstone and an Indiana limestone specimen are investigated through series of two-phase (water-N<sub>2</sub>) core-flooding experiments (i.e., drainage) under increasing effective stress from 10 MPa to 30 MPa and isothermal (40°C) conditions. We used X-ray computed micro-tomography to quantify changes in the topology of the pore-space with effective stress. The controls of the capillary number on the stress-dependent shifts of *Sw<sub>ir</sub>* is studied through experiments under constant injection rate and constant injection pressure conditions, independently. We find a 22% and 52% decrease in *Sw<sub>ir</sub>* of Berea sandstone and Indiana limestone, respectively, in response to an increase in effective stress under constant injection rate (i.e., increasing capillary number) condition. We further find a 27% increase in *Sw<sub>ir</sub>* of Indiana limestone with the same increase in effective stress under constant injection pressure (i.e., decreasing capillary number) condition. We reveal that the deformation of the pore throats, due to an excess effective confining stress, and changes in the driving energy for the gas phase to invade smaller channels, due to an increase/decrease in capillary number, leads to a decrease/increase in *Sw<sub>ir</sub>* of both specimens. These micro-scale and macro-scale observations underscore the remarkable control of capillary number on deformation-dependent fluid-fluid displacement in porous media, which pave the way for relevant research in geoscience and engineering.

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Haghi, A.H., Chalaturnyk, R., Blunt, M.J., Hodder, K., Geiger, S., (2020). Poromechanical Controls on Multiphase Fluid Flow in Earth Material. *Scientific Reports*, 11, 3328.

Haghi, A.H., Talman, S., Chalaturnyk, R. (2020). Consecutive Experimental Determination of Stress-dependent fluid flow Properties of Berea Sandstone and Implications for Two-phase Flow Modelling. *Water Resources Research*, 56(1)

Haghi, A.H., Chalaturnyk, R., Talman, S. (2019) Stress-Dependent Pore Deformation Effects on Multiphase Flow Properties of Porous Media. *Scientific Reports*, 9(1), 1-10 **Acceptance of Terms and Conditions:**

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## **Experimental Study on Long Core of Fractured Vuggy Metamorphic Rock Rich in Condensate Gas Reservoir with Different Development Methods**

**Authors:** Jinman LI<sup>1</sup> ; Jinze LI<sup>2</sup>

**Co-authors:** Hongbo HUO<sup>3</sup> ; Yang LIN<sup>2</sup> ; Linsong CHENG<sup>4</sup> ; Jinsheng SUN<sup>4</sup>

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BZ oilfield in Bohai Bay is a fractured porous metamorphic reservoir, which shows the characteristics of double porosity and double permeability. The mechanism of condensate reverse evaporation is also different from that of general sandstone condensate gas reservoir. In this paper, firstly, the metamorphic core without fracture was obtained for porosity and permeability test (average porosity 5.6%, average permeability 1.5md), and then the fracture (fracture permeability 5-10md) combination long core 108.6cm was carried out. Then, the depletion, gas injection, huff and puff and pulse gas injection experiments were carried out in this long core with condensate gas (condensate oil content 689g / m<sup>3</sup>) fluid to optimize and enhance condensate oil recovery The best way to develop. The experimental results show that the condensate recovery of depletion development is lower, the top depletion is lower than that of horizontal depletion, the condensate recovery of direct gas injection above dew point pressure is the highest, followed by direct gas injection or pulse gas injection under the maximum condensate saturation, which is different from the conventional low permeability sandstone condensate gas reservoir, and the effect of gas injection huff and puff is the worst. This experiment has a very good guiding significance for the reasonable development of high condensate oil-bearing condensate gas reservoirs in fractured vuggy reservoirs.

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## Experimental analysis and modeling of non-isothermal transient flows in granular porous media at large Biot numbers

**Author:** Cyril Levét<sup>None</sup>

**Co-authors:** Azita Ahmadi<sup>1</sup> ; Guillaume Bon<sup>2</sup> ; Hermes Scandelli ; Jean Lachaud<sup>3</sup> ; Shaolin Liu

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Numerous green technologies are based on heat and mass transfer in porous media at high temperatures : heat exchangers for thermodynamic solar power plants, biofuel production from biomass, etc.

This type of transfer often involves several non-Darcian effects such as inertial [1], compressibility and unsteadiness effects, and, most importantly, local thermal non-equilibrium effects between the gas and the solid [2] but also sometimes within the solid itself (high Biot number) [3]. Upscaling models have been proposed [4] and have shown to provide acceptable results for an intermittent energy storage system [5]. The complexity of real granular packings and coupled non-darcian effects with non-equilibrium heat transfer in the transient regime require experimental measurements to accurately identify homogenized model parameters. We have developed an experimental setup to measure the non-Darcian parameters in centimetric granular porous media. It consists of a 20 cm diameter, 1 meter long, tube filled with the granular porous medium of interest. Hot gas is blown at the required flow rate and temperature at the inlet of the tube (in the current version, up to 0.5 m/s and 800 K). The temperature evolution of the gas and of the grains are monitored during dynamic heating, steady state and cool-down.

Macroscopic models proposed in the literature [2, 4] have been implemented in the Porous Material Analysis Toolbox based on OpenFoam (PATO) [6], which is released Open Source (www.pato.ac). Parameter estimation is done using advanced multi-objective optimization, coupling Dakota [7] with PATO. This work illustrates the strategy and presents results in the case of a high temperature, compressible, inertial, and transient flow in a pebble packed bed.

### Time Block Preference:

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MS9 / 485

## Experimental and Numerical Study of the Dynamic Wetting influence on the Multiphase Flow in a Pore Doublet Model

**Author:** Amine Ben Abdelwahed<sup>1</sup>

**Co-authors:** Azita Ahmadi<sup>1</sup> ; Joël Bréard<sup>2</sup>

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Multiphase flow in porous media is a subject with important technical applications, such as in oil recovery from petroleum reservoirs or in Liquid Composite Molding Processes. In the Liquid Composite Molding and in other applications, macroscopic resin flow is modelled by postulating a multiphase generalization of Darcy's law. However, modelling of multiphase flow remains an important technical challenge and a thorough understanding of pore-scale physics and robust upscaling methods are of great importance.

This work addresses micropore-scale multiphase flow, in which different pressures are defined in each constituent phase with the differences, called capillary pressure, obtained by the micropore geometry and the interfacial tension. Consequently, the study of forces acting inside a fluid or at the interfaces liquid/liquid, liquid/vapor or liquid/solid is very significant to improve the understanding of multiphase flows in porous media [1, 2].

The aim of this work is to study the dependence between the contact-line velocity and the slip length in a Generalized Navier Boundary Condition (GNBC) [3, 4], by confronting numerical simulations to experimental data. Experiments were performed by a liquid/gas cross-flowing mechanism inside a pore T-junction device. For typically small capillary numbers (between 10E-6 and 10E-2) of the continuous shear stream, the dynamic contact angle is found to have a significant effect on the bubble size. This can be explained by the non-uniform displacement of the contact line at the solid wall. Computer fluid dynamics (CFD) simulations of dynamic wetting were performed using a slip model on the substrate. Realistic values of the slip length were chosen by matching the numerical dynamic contact angles obtained by the GNBC Model and experimental ones.

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Time Block B (14:00-17:00 CET) **References:**

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MS8 / 173

## Experimental investigation of buoyant convection in a heterogeneous porous media: Two-layers separated by an inclined permeability jump\*

**Author:** K. S. Bharath<sup>1</sup>

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In this study, we employ a ‘filling-box’ model to experimentally investigate the flow of a dense, Boussinesq plume through a saturated porous medium characterized by a high permeability layer above and a low permeability layer below. The boundary, or permeability jump, separating the two layers is inclined to the horizontal. Upon striking the permeability jump, the discharged plume fluid propagates along the permeability jump as an unequal pair of up- and down-dip ‘primary’ gravity currents. As these gravity currents propagate, some fluid is lost by drainage through the permeable boundary. The associated (early time) spreading behavior has been theoretically investigated in our previous work (Bharath *et al.*, *J.FluidMech.*, **902**, 2020). It was shown that the primary gravity current reaches runout (static state), wherein inflow from the plume is precisely matched by outflow due to draining. This static state can be maintained only so long as the discharged plume fluid falling through the lower layer does not itself collide with an impermeable boundary. Once such a collision occurs, there will form a pair of ‘secondary’ gravity currents, which, in turn, exert a significant dynamical influence over the entire depth of the heterogeneous porous medium. For instance, the secondary gravity currents will “tug” upon the primary gravity currents leading to a remobilization of this previously-arrested front. At later times, primary and secondary gravity current flows are impeded by vertical sidewall boundaries. In characterizing the resulting filling-box flow, we distinguish between two qualitatively different filling regimes, i.e., a sequential vs. simultaneous filling of upper- and lower-layers with contaminated fluid. Parameter combinations conducive to one or the other filling regime are also identified.

Through this work we attempt to address some of the key uncertainties in the field of underground hydrogen storage and carbon-dioxide/acid-gas sequestration. These uncertainties include (i) the degree of asymmetry in the flow structure of the gravity current pairs as they propagate along an inclined and permeable boundary, (ii) the influence of impermeable boundaries encapsulating the porous media, and, (iii) the nature and time required to fill the porous medium in the presence of heterogeneities.

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\*Funding Acknowledgment: NSERC **Acceptance of Terms and Conditions:**

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## **Experimental investigation of physical dispersion and in-situ mixing during low salinity waterflooding**

**Author:** Arman Darvish Sarvestani<sup>1</sup>

**Co-authors:** Behzad Rostami<sup>1</sup> ; Hassan Mahani<sup>2</sup>

<sup>1</sup> *University of Tehran*

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Low salinity waterflooding (LSWF) as an enhanced waterflood technique is applicable in secondary and/or tertiary oil production. The performance of LSWF depends on different factors including the volume of injected brine, its salinity and in-situ mixing. Mixing is intensified due to adverse mobility ratio at low salinity (LS) - high salinity (HS) front. This research focuses on the impact of salinity of

injection and resident brine (salinity gradient) on physical dispersion through single-phase (miscible) sandpack tests.

A systematic series of single-phase sandpack tests were performed. In this manner, the sandpack was initially saturated with high salinity brine (HS) and flooded with low salinity brine (LS), afterward. Consequently, the initially uniform salt distribution in the sandpack was altered gradually, leading to development of salinity gradient and mixing zone in the sandpack. The salinity of the effluent brine was measured as a function of injected pore volume. A coherent analytical approach was then carried out to estimate the length of mixing zone with respect to Peclet number and dispersivity. The salinity difference of the brines used in the tests were between 36,000 to 156,000 ppm.

It was observed that dispersivity and physical dispersion of salt during LSWF depends on the salinity of HS and LS. The higher the salinity difference, the higher the dispersivity. The maximum estimated dispersivity was observed for a test in which the salinity of HS and LS were 160,000 and 4,000 ppm, respectively. The estimated dispersivity of this test was 0.0071 ft. which is equivalent to a Peclet number of 116. The minimum dispersivity was obtained when the salinity difference was 36,000 ppm. The dispersivity of this test was estimated to be 0.0040 ft. which means the Peclet number is increased to 205. Putting all results together, it can be concluded that for a system with lower salinity difference, lower volume of LS will be required to establish low salinity conditions throughout the porous system.

The impact of salt concentration of resident HS and LS injection brine on physical dispersion/mixing of brines with different salinity was experimentally investigated for the first time, to the best of our knowledge. Moreover, visual evidence was provided to discuss the impact of salinity and salinity difference of brines on dispersivity of the system.

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## **Experimental study of drying in the presence of fluorescent colloidal particles in model porous media**

**Authors:** Elisa Ghiringhelli<sup>None</sup> ; Marc Prat<sup>None</sup> ; Manuel MARCOUX<sup>1</sup>

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The motivation for the present study stems from visualizations of the PTFE distribution in the gas diffusion layer (GDL) of Proton Exchange Membrane Fuel Cell (PEMFC). The GDL is a fibrous carbon layer treated with polytetrafluoroethylene (PTFE), by drying a layer saturated with a solution of PTFE particles, to improve hydrophobicity [1, 2, 3]. During the fabrication, internal surfaces appears to be hardly covered homogeneously causing a mixed wettability in the medium, indeed it is showed in [4] that PTFE distribution strongly depends on evaporation conditions, such as the surrounding pressure. In this context, the objective of the work is to study the pattern formed by fluorescent colloids (250nm) in the porous media after the evaporation of the water, in different geometries, starting from a single pore before moving to a pore network on micro-models and/or with different initial conditions. The first step was to use a transparent material to make the porous medium (polymer), filling it with a solution of fluorescent red colloids and let it dry at constant temperature and humidity. Using fluorescent colloids allows us to visualize the final particle deposit. With this type of particles, it will be also possible to follow their position during evaporation, compute the velocity field and connect it to the final deposit. The flow of water during evaporation and the pattern of deposited particles were observed under a microscope using a confocal green source. In the pictures below the particles are bright.

The largest channel is the first one to dry out, forcing the particles to move on the other side. This results in an overall heterogeneous pattern of deposited particles, with higher concentration in the narrower channel, see Figure (d). The experiment also indicates that the evaporation of the residual liquid films at the very end of the drying process do have an impact on the final particle deposit.

The next step is to be able to analyse and predict the materials properties such as wettability, contact angle, hydrophobicity of particles, etc...on polymer micromodels. These procedures would allow us to explain how the fluid moves while drying, thanks to the tracking of particles, how it influences the colloidal particle deposition and finally, find procedures to improve GDL's hydrophobicity properties for better fuel cell operation.

Figure: (a), (b) and (c) different stages of evaporation in a plexiglass pore 3mm x 3mm filled with a solution with concentration  $2 \times 10^{-5}$  % (timesteps: 20 minutes, 1 hour and 40 minutes and 3 hours), (d) deposit of the bright particles after drying.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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MS6-A / 653

## Experimental study of steady state flow paths during the immiscible flow of ganglia in stochastic porous media micromodels

**Author:** Athanasios Anastasiou<sup>1</sup>

**Co-authors:** Ioannis Zarikos<sup>1</sup>; Andreas Yiotis<sup>2</sup>; Laurent Talon<sup>3</sup>; Dominique Salin<sup>3</sup>

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Immiscible two-phase flow in porous media is a physical process encountered in a wide variety of applications, such as oil recovery, soil remediation, CO<sub>2</sub> sequestration, as well as in several industrial systems. The models that describe two-phase flow in such porous media are traditionally based on Darcy's law and are typically valid when both phases are continuous over the entire flow domain. Under several flow conditions, however, one of the fluid phases is discontinuous (typically the non-wetting one) and moves under the effects of shear viscous stresses and pressure gradients imposed at its interface by the continuous (typically wetting) phase. The movement of the discontinuous phase in the form of ganglia has been the subject of various studies (1–4), with existing theories being formulated on the basis of data, which analyze the phenomenon based on the overall movement of

the ganglia.

In this work, we study experimentally the flow of non-wetting phase ganglia during the co-injection of oil and water in a predominantly 2D PMMA micromodel. The micromodel is constructed using a CNC milling machine based on a stochastically reconstructed digital pattern that generates randomly shaped pillars of solid that follow a Gaussian size distribution. The flow is recorded using a high-resolution DSLR and the resulting images are post-processed to obtain both the ganglia size distributions and the temporally-averaged distribution of phases. We thus identify the effects of the flow rate (controlled by two rotary pumps) and the viscosity ratio of the fluids (by selecting oils of various viscosities) on the steady-state ganglia size distributions, the ratios of mobile over stranded ganglia phase saturation and the density of the flow paths, where the transport of the disconnected phase takes place. Our results demonstrate that the rates of ganglia fragmentation and coalescence intensify at higher Ca values, leading to size distributions that shift towards smaller average values. This effect can be directly correlated with the emergence of new flow paths that develop through narrower pores-throats as viscous forces progressively become dominant over capillary ones. The flow of ganglia through these narrower pores leads to their snap-off and fragmentation into smaller sizes.

#### Time Block Preference:

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MS6-A / 227

## Experimental study of the contact angle of hydrogen-brine-rock for subsurface energy storage

**Authors:** Leila Hashemi<sup>1</sup> ; Wuis Glerum<sup>1</sup> ; Rouhi Farajzadeh<sup>2</sup> ; Hadi Hajibeygi<sup>1</sup>

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Feasibility of underground hydrogen storage (UHS) as a promising large-scale energy storage has become an attractive subject in recent years. Geological formation such as aquifers, depleted oil and gas reservoirs and salt caverns provide giant capacities for hydrogen storage. Compared with salt caverns, geological porous rock reservoirs (including aquifers and depleted hydrocarbon reservoirs) provide much larger volumes. However, successful utilisation of porous reservoirs for hydrogen storage depends on accurate characterisation of hydrogen transport at pore-scale which is to a large extent unknown. The pore-scale characteristics, such as contact angle, play crucial role in determining upscaled parameters such as relative permeability and capillary pressure curves. These functions will be then used to perform modelling and optimisation at reservoir scale.

In this study, for the first time, we characterise the contact angle of hydrogen in contact with brine and subsurface geological rocks at pore scale. We utilise a captive bubble method, which allows for controlled-injection of hydrogen at a given pressure and temperature; to form accurate bubbles in a



fully saturated environment. The experiments are conducted in a hydrogen-brine-sandstone system close to UHS in-situ conditions. More precisely, pressure is changed between 0 – 100 bars and temperature between 20 – 50 °C. Also, an axisymmetric drop shape analysis-profile (ADSA-P) method is used to measure contact angles. First, we validate the setup for the published results in the literature for N<sub>2</sub> gas, and then introduce H<sub>2</sub> and report the accurate contact angles along with quantified errors and uncertainty range. The study is the first of its kind and will result in accurate Kr and Pc curve definitions for reservoir-scale analyses of hydrogen storage in subsurface formations.

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MS3 / 372

## Experimental study of water vapour condensation in cracked concrete with different specimen states visualised by neutron tomography

**Author:** Ritesh Gupta<sup>1</sup>

**Co-authors:** Bratislav Lukić<sup>2</sup> ; Alessandro Tengattini<sup>3</sup> ; Matthieu Briffaut<sup>4</sup>

<sup>1</sup> *Post-doctorant*

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This work provides new experimental evidence regarding two-phase fluid flow in damaged porous media. The results aim to provide novel cases towards leakage rate modelling dedicated to the well-prediction of reliability and durability of the pressurised concrete structures such as nuclear containment buildings.

Previous experimental works on the structural scale, e.g. reinforced concrete slabs tested at MPA Karlsruhe<sup>1</sup> and in MAEVA model<sup>2</sup> show that the air-vapour leakage rate is lower than the leakage rate of dry air. The accurate prediction of the complex interplay of multi-physics phenomena necessitates the use of sophisticated numerical models. The adaptation of such models demands the calibration and validation in simple yet realistic experiments whose thermo-hydric boundary conditions are well-defined.

With this regard, we present an experimental study, where, here a well-controlled flux and saturation of the hot-steam and air mix is injected through a cracked cylindrical concrete specimen of diameter and length 40mm. Brazilian test is conducted on the specimen, equipped with LVDTs on both circular faces, to create  $\approx 150\mu\text{m}$  crack opening displacement (COD). The required COD is achieved by progressive crack opening with several loading/unloading cycles.

Dry and saturated cracked specimen states, representative of the in-situ limiting conditions, are examined for interaction with the injected vapour. Temporal evolution of temperature and pressure at both specimen boundaries are recorded and the whole process is visualised with sequential in-operando neutron tomographies of 30secs. The speed of vapour travel along the crack is reported higher for saturated specimen state in comparison to the dry state. The capillary suction around the crack is prominent for dry specimen and comparatively negligible for the saturated specimen. A relationship between the material microstructural damage and the vapour flow is presented with emphasis on the initial state of saturation in the specimen.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

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Poster + / 46

**Explicit simulation of seismic waves in fluid-filled fractured porous media****Authors:** Vasily Golubev<sup>1</sup> ; Alexey Shevchenko<sup>1</sup><sup>1</sup> *Moscow Institute of Physics and Technology***Corresponding Authors:** alexshevchenko@phystech.edu, w.golubev@mail.ru

Oil and gas deposits are still the largest energy sources among all over the world. The most common and reliable method of their prospecting and exploration is the seismic survey process. It is based on the propagation of seismic waves in geological media and their interaction with heterogeneities (reflection, diffraction, attenuation). Recently, a lot of migration and inversion algorithms were developed: full-waveform inversion, petrophysical inversion, stochastic inversion, etc. All of them are based on the numerical solution of the direct wave problem. That is why, the investigation of accurate and effective methods of the computer simulation is an important scientific task.

Previously, the usage of sophisticated mechanical-mathematical models for describing the dynamic behavior of geological media was strictly limited by the performance of available computers. In the last century, several models describing wave propagation in porous fluid-saturated media were proposed. Initially, the Gassmann model [Gassmann, 1951] has become widespread. Further, the Biot model [Biot, 1956], has grown more popular, since it describes the porous medium more accurately. For example, the Biot model considers two velocities of longitudinal waves that can be observed and measured experimentally [Winkler et al., 1989]. In 1989, V.N. Dorovsky proposed a non-linear continual theory of filtration [1989]. The theory was expanded in the work [Blokhin and Dorovsky, 1995], and the two-velocity linearized model, known now as the Dorovsky model, was presented. The comparison of the continuum filtration theory with the Biot-Johnson theory was done at [Dorovsky et al., 2012]. Both models show excellent agreement with each other. Another physical model of the multiphase medium was suggested in [Romensi et al., 2019]. Its governing equations form a hyperbolic system of PDEs that significantly differs from the Biot system [Biot, 1956] because of the different stress-strain relationships; however, the authors state that “the features of wavefields are qualitatively similar in both models, and in some cases, they are quantitatively close by a corresponding choice of the material parameters” [Romenski et al., 2019].

In this work we extended our novel approach for the simulation of seismic waves in hydrocarbon deposits [Golubev et al., 2020] to the case of fractured fluid-saturated medium described by the Dorovsky model. We relied on the method of incorporating fractures into the computation process presented in [Khokhlov et al., 2020] for isotropic elastic media, which replaces an inclined fracture with a number of small fractures tied to the mesh points and duplicates the corresponding nodes (containing the unknown functions). The feature of the method is the possibility to perform calculations on a structural computational grid, that avoids the construction of unstructured grids and

drastically decreases computational costs. Physically correct internal contact conditions were derived for the two sides of the fracture, that eliminates the meshing process inside the crack volume. The presented approach allows us not only to simulate precisely the stress-strain state, but also to estimate the pore pressure inside the reservoir.

The reported study was funded by RFBR, project number 20-01-00261.

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Time Block A (09:00-12:00 CET) **References:**

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**Poster + / 820**

## **Extending a low permeability fluid flow model for transient flow of compressible and slightly compressible fluids.**

**Author:** Susan Schrader<sup>1</sup>

<sup>1</sup> *Montana Tech*

**Corresponding Author:** [sschrader@mtech.edu](mailto:sschrader@mtech.edu)

Darcy's Law, an important equation relating flow velocity in a porous medium to the permeability of the medium and the viscosity of the fluid, can be extended to form flow models for petroleum fluids in a reservoir by combining it with a fluid model and conservation of mass. The resulting models are central to reservoir engineering. Analytic solutions to these flow models, developed by Van Everdingen and Hurst, are used in well testing and water influx calculations and their numerical solutions form the basis of many reservoir simulation programs.

However, as interest grows in low permeability reservoirs, Darcy's Law might not be the appropriate starting place. Alternatives to Darcy's Law include include threshold pressure models and nonlinear pressure models [1]. In this work new flow models are developed by combining these alternatives with conservation of mass, various fluid models and bulk/boundary fluid viscosity models [2].

Future work will involve using finite difference methods to develop numerical simulations of these models to compare to conventional simulation and historical data in petroleum and CO<sub>2</sub> sequestration applications.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

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MS9 / 484

## Extending equilibrium thermodynamics to include fluid-surface interaction for nanonconfined fluids

**Author:** Narendra Singh<sup>1</sup>

**Co-authors:** Filip Simeski<sup>1</sup> ; Matthias Ihme<sup>1</sup>

<sup>1</sup> *Stanford University*

**Corresponding Authors:** filip.simeski@stanford.edu, mihme@stanford.edu, narsingh@stanford.edu

For nanoconfined fluids, equilibrium properties such as adsorption, density, and surface diffusion are dependent on the layered structure of the fluid near the surface. This layered structure is also relevant to describe transport as the noncontinuum effect, such as slip velocity, depends on the near-wall density. While molecular dynamics simulations quantify the layered density profile in nano-configurations, a systematic theoretical development to calculate equilibrium properties remains challenging. We consider a grand canonical ensemble and include fluid-surface interaction exclusively in the configurational integral. Using Lennard-Jones type interaction between the fluid and surface in the configurational integral, an approximation to the grand partition function for confined fluid is derived. Theoretically obtained density profiles are compared with grand canonical Monte Carlo simulations. While the focus of the present work is the density of the fluid, other static equilibrium properties and transport related quantities such as correction to slip can be derived using the surface-interaction corrected partition function.

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Poster + / 195

## Extension of SAFT equation of state to include calcite wall effect in water properties within water-calcite interface using molecular dynamic simulations

**Author:** Sajjad Ahmadigoltapeh<sup>1</sup>

**Co-authors:** Saeed Abdollahi<sup>2</sup> ; Helge Hellevang<sup>1</sup> ; Miri Rohaldin<sup>3</sup>

<sup>1</sup> *University of Oslo*

<sup>2</sup> *Amirkabir University of Technology*

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On the fluid-rock interface, the order of the molecular structure and dynamical properties of fluid deviates from that of the bulk phase and the fluid exhibits a different thermodynamic behavior. To develop an understanding of the fluid-rock interface molecular dynamic (MD) simulation is conducted for water-calcite system. In this study, the results of MD simulations explicitly exhibit the layering transition of water on water-calcite interface. To predict the water properties near calcite wall, we have defined a contribution for Helmholtz energy extended from SAFT equation of state (EOS). In this approach, the confined water molecules interact with calcite surface through a square well energy ( $\epsilon$ ) estimated by MD simulation at a certain temperature (T). The outcomes of MD simulations confirm the fluctuation of energy, within the confinement, corresponds to the the calcite electrostatic field on the bulk water. The modified SAFT shows a good agreement with MD observations and the introduced model can predict the thermodynamic properties of water at systems with low water content.

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MS12 / 775

## FEM Modeling of Spherical Indentation in a Poro-elasto-plastic Medium

**Author:** Haiying Huang<sup>1</sup>

**Co-author:** Ming Liu<sup>1</sup>

<sup>1</sup> *Georgia Institute of Technology*

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Poroelastic spherical indentation via step displacement loading has been applied in the literature as an experimental technique to characterize poroelasticity. In theory, for a fully saturated porous medium with incompressible constituents, if the indenter is subjected to step displacement loading, elastic constants can be determined from the early and late time responses according to the Hertzian contact solution, while hydraulic diffusivity or the coefficient of consolidation can be obtained from the transient response by matching the measured indentation force as a function of time against a master curve.

Our previous theoretical works have shown that for porous media with compressible constituents, such poroelastic master curves can be constructed for three distinct types of surface drainage conditions, namely, case I - a fully permeable surface, case II - a fully impermeable surface and case III - a mixed drainage condition where the surface is impermeable in the contact region, but permeable everywhere else. These master curves have only weak dependence on material properties through a single derived parameter. However, for geomaterials such as soils and rocks, yielding and tensile fracturing may occur if the indentation depth exceeds a threshold. Understanding how

plastic deformation and tensile failure affect the spherical indentation process is therefore crucial to establishing spherical indentation as an experimental technique for poroelasticity characterization of geomaterials.

In this work, a fully coupled finite element analysis is conducted to investigate the poro-elasto-plastic spherical indentation process. We show that hydromechanical coupling gives rise to four distinct types of poro-elasto-plastic responses. Even though plasticity occurs immediately at the undrained limit, if cohesion is within a certain threshold, there is no plastic strain accumulation during the transient phase. The normalized force relaxation behavior could still be approximated as poroelastic. Insights gained from this numerical analysis therefore could be valuable in supporting the use of spherical indentation for poroelasticity characterization for geomaterials.

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## **FLEXT – A Flexible Scripting X-ray Computed Tomography System for Multiscale and Dynamic Imaging of Porous Materials**

**Authors:** Armin Afrough<sup>1</sup> ; Karen L. Feilberg<sup>1</sup>

<sup>1</sup> *Centre for Oil and Gas – DTU, Technical University of Denmark*

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X-ray Computed Tomography (CT) methods can be employed to study the internal structure of porous geomaterials non-destructively and with minor sample preparation. Previously, such methods have been utilized in the characterization of petroleum reservoirs, underground water resources, soil, and carbon storage in aquifers. X-ray CT has the potential to characterize porous geomaterials at multiple length scales and as a function of time – in the dynamic imaging mode. Multiscale and dynamic imaging of geomaterials in X-ray CT scanners however requires open hardware and software architectures that permit programming, scripting, and modifications.

We developed a flexible scripting software system in MATLAB to control the components of a non-commercial multiscale X-ray CT scanner for geological applications. The modified custom-built X-ray CT scanner is capable of imaging objects as large as 20 cm to smaller than 1 mm. The flexibility of the software and hardware permitted the placement of three rotation stages in the scanner to image a variety of samples. Many rock samples from chalk reservoirs of the Danish North Sea, on the 120-mm, 40-mm, and 2-mm length scales, were imaged and demonstrated the multiscale capabilities of the developed imaging system. Millimeter-sized, core plug, and whole core samples demonstrated the possibility of observation of a range of features, including fossils, fractures, pyrite agglomerates, pores and holes, deformation bands, and stylolites across different length scales.

A flexible imaging software system is necessary to accelerate the time resolution of dynamic imaging by algebraic iterative reconstruction or time-discrete Kalman filter algorithms. The software system developed in this work can acquire projection images at any order of angles, or combination of other stage positions, according to user input. In simple cases of full circular cone-beam datasets, all angular data are acquired in series and the same rotation pattern is repeated over time. Two dynamic evaporation experiments in a model glass-bead pack and a natural chalk core plug demonstrated the dynamic capabilities of the scanner. In evaporation of deionized water in a glass bead pack, water evaporated over the course of more than 3 days and left pendular rings behind. The evaporation of

saltwater from a 3.9-mm-diameter Stevns Klint chalk plug demonstrated the possibility of observing efflorescence, the formation of a crystallized salt layer on the porous medium, and changes in the liquid phase content through partial volume effects.

Flexible X-ray CT systems such as the one described in this work provide opportunities to easily and quickly learn and modify existing imaging protocols and add new layers of hardware and software to explore new ideas.

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## Fabrication of Reactive Rocks with 3D Printing

**Authors:** Shelby Wales<sup>1</sup> ; Ishan Anjekar<sup>2</sup> ; Vinita Shinde<sup>1</sup> ; Bryan Beckingham<sup>1</sup> ; Lauren Beckingham<sup>2</sup>

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The heterogeneity of natural geologic samples presents significant challenges in furthering our understanding of geochemical reactions in porous media. This investigation explores the feasibility of fabricating reactive rocks through novel additive manufacturing techniques by integrating reactive materials with polymer filaments. Using 3D X-ray Computed Tomography (X-ray CT) images of a sandstone sample from the Paluxy formation in Mississippi, a template was created to 3D print a model of the system's pore structure. Two methods for fabricating a rock structure consisting of a reactive phase that reflects the properties of the real sample are investigated here. The first method entails mixing calcite particles with HIPS pellets and extruding a customized reactive filament. The second method consists of dispersing calcite in THF and using the resultant mixture to coat segments of HIPS filament. The filaments were used to 3D print models, and the relative success of each method was evaluated via by optical microscopy, 2D Scanning Electron Microscopy, and 3D X-ray CT imaging. For each set of images, calcite volume fractions and the exposed calcite surface area are determined using ImageJ and MATLAB. Results from the first method indicate that calcite surface areas are comparable to real samples, albeit most of the calcite is inaccessible. This will be compared with accessible surface areas of samples printed with the calcite coated filament. These findings will be used to inform further pathways for utilizing 3D printing as a means of modelling reactive porous media in pursuit of a solution that accurately reflects the pore structure and reactive properties of real samples.

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MS1 / 245

## Fault permeability and rupture in injection-induced earthquakes

**Authors:** David Santillan<sup>1</sup> ; Ruben Juanes<sup>2</sup> ; Juan Carlos Mosquera<sup>1</sup> ; Luis Cueto-Felgueroso<sup>3</sup>

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Injection-induced seismicity has arisen as a central concern in the development of subsurface energy technologies such as enhanced geothermal energy, unconventional hydrocarbon production, wastewater injection, geologic carbon sequestration, or underground gas storage. The effect of the hydraulic properties of faults on the rupture of injection-induced earthquakes is still poorly understood.

Here, we study the effect of the hydraulic properties of faults on the rupture of injection-induced earthquakes. The hydraulic properties can range from sealing to complete conductive, both in terms of flow along and across the fault. Our research question is how these properties may alter the onset of slip, the symmetry of the rupture process, or the magnitude of the earthquake in terms of the seismic moment.

We simulate earthquakes through sophisticated two-dimensional computational models where events are triggered by fluid injection. We describe the fault frictional contact with the Dieterich-Ruina rate-and-state law. Rock is simulated as a poroelastic solid and we couple fluid flow and rock mechanics. Our approach lets us quantify the impact of longitudinal and transverse fault permeability on the mechanisms that control the evolution of fault strength and shear stress during the rupture. We find that fault permeability drives fault stress and strength states at the onset of the rupture, and these in turn control the magnitude of the subsequent earthquake. Therefore, fault permeability exerts a fundamental control on the magnitude of earthquakes.

**Acknowledgments:** Project supported by a 2019 Leonardo Grant for Researchers and Cultural Creators, BBVA Foundation. The BBVA Foundation accepts no responsibility for the opinions, statements, and contents included in the project and/or the results thereof, which are entirely the responsibility of the authors.

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Poster + / 571

## Feedback mechanisms between precipitation and dissolution reactions across randomly heterogeneous conductivity fields

**Authors:** Alberto Guadagnini<sup>1</sup> ; Giovanni Porta<sup>1</sup> ; Martin Stolar<sup>2</sup> ; yaniv edery<sup>2</sup>

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Our study aims at investigating the interplay between the dissolution, precipitation and transport processes taking place within randomly heterogeneous conductivity domains and the ensuing spatial



distribution of preferential pathways. We do so by relying on a collection of computational analyses of reactive transport performed across two-dimensional systems where the (natural) logarithm of conductivity is characterized by various degrees of heterogeneity. Our results document the joint occurrence of precipitation and dissolution. While the latter mainly takes place along preferential flowpaths associated with the generated conductivity fields, the former is observed at locations close to and clearly separated from these. The high conductivity values associated with the preferential flowpaths tends to further increase in time, giving rise to a self-sustained feedback between transport and reaction processes. The clear separation between regions where dissolution or precipitation takes place is imprinted onto the sample distributions of permeability which tend to become visibly right skewed (with a tendency to bimodality) with time. The link between conductivity changes and reaction-driven processes promotes the emergence of non-Fickian effective transport features. The latter can be captured through a continuous time random walk model where solute travel times are approximated with a truncated power law probability distribution. The parameters of such a model are seen to change with time, shifting towards values associated with increasingly high non-Fickian effective transport behavior.

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## Film entrainment and particle transport during gas invasion in suspension-filled microchannels

**Author:** ting wu<sup>1</sup>

**Co-authors:** ran hu<sup>2</sup>; hua zhong<sup>3</sup>; lei yang<sup>4</sup>; wenbiao jin<sup>4</sup>; yifeng chen<sup>5</sup>; zhibing yang<sup>3</sup>

<sup>1</sup> Wuhan University

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Displacement of particle suspension by air is ubiquitous in nature where the particle transport plays an important role in the displacement process. Here we experimentally study the film entrainment and particle transport during gas-suspension displacement in microchannels. We characterize three flow regimes, ranging from no deposition to particle entrapment and to particle layering within liquid films, depending on the withdrawal rates and the particle volume fraction in the suspension. The film thickness is shown to be dependent on a modified capillary number  $Ca_0$  which takes into account the effects of flow velocity, particle volume fraction, and channel shape and effectively captures the general behavior of microplastics entrainment for particle volume fraction in the range of 0~20%. A theoretical prediction of the critical capillary number  $Ca_0^*$  for particle entrainment is found to be consistent with the experimental results. The probability of entrainment for particles near the gas invading front is found to be proportional to both particle volume fraction and the capillary number. This work elucidates the mechanism responsible for the effect of suspended microplastics on immiscible displacement in confined geometries and is of practical importance in many natural and engineered applications spanning from environmental systems to microfluidics and geophysical flows.

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Poster + / 421

## Filtration with multiple species of particles

**Authors:** Yixuan Sun<sup>1</sup> ; Lou Kondic<sup>2</sup> ; Linda Cummings<sup>2</sup>

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Membrane filtration with a feed containing multiple species of particles is common in the industrial setting and many experimental results are available; however, little theoretical work in terms of first-principles mathematical modeling has been reported. We propose a simplified model for filtration of a suspension containing an arbitrary number of particle species, each with different affinities for the filter membrane. We use our model to formulate and solve selected optimization problems for the filtration of a feed solution containing two particle species, where one is to be removed by the filter and the other retained in the filtrate. In addition, we investigate the screening (shielding) effect, which is thought to contribute to the particle retention deterioration observed in experiments over the lifetime of a filter.

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MS24 / 224

## Fixed Stress Splitting for Coupled Flow and Poromechanics

**Authors:** Mary Wheeler<sup>None</sup> ; Xueying Lu<sup>1</sup> ; Vivette Girault<sup>None</sup>

<sup>1</sup> *UT Austin*

**Corresponding Authors:** girault@ann.jussieu.fr, xyly@utexas.edu, mfw@ices.utexas.edu

Professor Andro Mikelić is known for his seminal mathematical contributions to flow in porous media. In this presentation we summarize how his work has impacted the development of numerical models coupling flow and poromechanics arising in geosciences and biosciences applications such as subsidence events, carbon sequestration, groundwater remediation, hydrocarbon production, and hydraulic fracturing, enhanced geothermal systems, solid waste disposal, and biomedical multiple-network poroelastic theory MPET modeling. We focus on the Biot model that consists of a poromechanics equation coupled to a flow model with the displacement and pressure as unknowns. In contrast to solving the Biot system fully implicitly, we consider a fixed stress iterative scheme that allows the decoupling of the flow and mechanics equations. The decoupling scheme offers several attractive features such as the use of existing flow and mechanics codes, use of appropriate preconditioners and solvers for the two models, and ease of implementation. The design of this approach is

currently quite popular in engineering studies due to its importance in the formulation of efficient, convergent, and robust schemes. Professor Mikelić's work on establishing a contractive property of this and several other iterative schemes has led to many theoretical and computational practical extensions, one of which we discuss in detail.

In this presentation we discuss the Biot system solved with a fixed-stress split, Enriched Galerkin (EG) discretization for the flow equation, and Galerkin for the mechanics equation. Residual-based a posteriori error estimates are established with both lower and upper bounds. These theoretical results are confirmed by numerical experiments performed with the Mandel's problem. The efficiency of these a posteriori error estimators to guide dynamic mesh refinement is demonstrated with a prototype unconventional reservoir model containing a fracture network.

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MS9 / 34

## Flow behavior in a rough channel with pore scale simulation

**Author:** Chao Xu<sup>None</sup>

**Co-authors:** Lei Zhang<sup>1</sup>; Guangpu Zhu<sup>2</sup>; Hai Sun<sup>2</sup>; Yongfei Yang<sup>2</sup>; Jun Yao<sup>2</sup>

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**Abstract:** Pore scale immiscible displacement is crucial in oil industry. The surface roughness of throat is an important factor affecting water-oil interface movement. In this paper, the Navier-Stokes (N-S) equation coupled with the phase field method is adopted to analyze the oil-water flow and interface movement in single channel, considering different surface roughness, diverse wettability and various capillary numbers. The simulation results show that the existence of asperities strengthens the interface deformation and promotes the formation of fingering phenomenon. The water-flooding process presents different flow patterns in the rough channel with diverse wettability, and the influence of wall roughness on oil-water interface movement is different under various wettability conditions. There is an approximate exponential relationship between the ratio of interface length to channel length and capillary number. Moreover, the influence of wall roughness on wettability can not be ignored. The threshold Ca number of the wall from water wet to oil wet was studied at diverse roughness heights and distributions, and different viscosity ratios were considered.

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MS3 / 124

## Flow in deformable fractures - From numerical studies to experimental investigations

**Authors:** Patrick Schmidt<sup>1</sup> ; Dongwon Lee<sup>1</sup> ; Matthias Ruf<sup>2</sup> ; Holger Steeb<sup>3</sup> ; Jörg Renner<sup>4</sup>

<sup>1</sup> *University of Stuttgart*

<sup>2</sup> *University of Stuttgart - Institute of Applied Mechanics (CE)*

<sup>3</sup> *Universität Stuttgart*

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Analysis of consistent experimental sets of hydro-mechanical data recorded during hydraulic experiments on single fractures or fractured reservoirs require a consistent numerical model to determine fracture properties with a high accuracy. Hence, this work briefly discusses the derivation and numerical implementation of a consistent, fully coupled hydro-mechanical model for flow in deformable fractures. The computational efficiency of the model is demonstrated in a complex fracture network setting in three dimensions before specific hydro-mechanical phenomena are discussed. One prominent phenomenon is the occurrence of overtones in the frequency domain recorded during harmonic excitation tests and their dependence on the specific normal stiffness characteristic of a single fracture. The relevance of the numerical findings for experimental investigations is demonstrated on different scales consulting results obtained from laboratory and in-situ field tests. Laboratory studies have been performed on single fractures embedded in a cylindrical sample using a recently designed triaxial set-up and transient in-situ measurement data was recorded during harmonic excitation tests at Reiche Zeche underground research laboratory.

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## Flow instabilities of viscoelastic polymer solutions in multiple contraction channels

**Author:** Eseosa Ekanem<sup>1</sup>

**Co-authors:** Steffen Berg<sup>2</sup> ; Shauvik De<sup>3</sup> ; Ali Fadili<sup>4</sup> ; Paul Luckham<sup>1</sup>

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Hydro-soluble polymer solutions are used in porous media for a range of applications from, enhanced oil recovery, ground water remediation and as permeability modifiers in oil reservoirs. During flow of these polymer solutions in porous media, shear viscosity dominates at low and intermediate shear rates, with the polymer solution undergoing a transition from Newtonian to shear-thinning behaviour. However, at high shear rates, the most commonly used synthetic type of polymer exhibits large unstable flows. Previous research in single contraction channels, representing one pore body-pore throat system of a porous medium, have shown that the unstable flows were due to the viscoelasticity of the polymer solution, coupled with the contraction in the microchannel, exhibiting high normal stresses at elevated strain. However, in the presence of multiple pore throats, such as in a porous medium, where there is interaction between different pore throats, the cause and effect

of the unstable flows generated need to be fully understood.

Therefore, in this work, we investigate the behaviour of purely elastic flow instabilities of viscoelastic polymer solutions generated in a multiple contraction microfluidic channel. We use micro-channels with throats that are separated by different channel lengths and having contraction ratios, CR, of 5 and 10. Also, we use a time resolved particle imaged flow velocimetry technique, to study the flow behaviours at low fluid inertia and we evaluate the M stability criterion, which predicts the onset of elastic instability. Results showed that flow instabilities, which are elastic in nature, were present above the critical M value. Consequently, we draw conclusions on the effect of the throat separation distance on the flow instabilities.

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MS16 / 737

## Flow of DNA solutions around cylindrical arrays

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Complex fluid responses to external forces, imposed at specific lengthscales and forcing amplitudes, are intimately linked to their internal microstructure. Accordingly, microstructure deformation and relaxation history span lengthscales from the microscale to the macroscale. When complex, biological fluids are driven through porous media, a faithful model of the trapped vs. transported fluid mixture, and whether the material remains intact or preferentially separates (a version of material failure), is strongly dependent on multiple interacting chemical and transport processes. These dynamics processes are consequences of properties of the porous medium, the biological fluid, the relative lengthscales of the pore structure and the complex fluid, and medium-fluid component affinities. If the porous medium is fibrous with relative stiff fibers, a “simple” first step is to understand how the fluid behaves around a sphere or a cylinder. We start with a lambda-DNA solution to illustrate how complex even this simple model problem is, with a wide range of behavior. This study is a first step in our main goal of proposing an experimental strategy and analysis of the experimental data to learn the dominant mechanisms governing transport of complex fluids through porous media, and to build a predictive model.

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MS6-B / 241

## Flow patterns and interface stability during drainage of liquid–particle mixtures

**Author:** Dongqi Li<sup>1</sup>

**Co-authors:** Zhibing Yang<sup>1</sup>; Renjun Zhang<sup>1</sup>; Ran Hu<sup>1</sup>; Yi-Feng Chen<sup>1</sup>

<sup>1</sup> *Wuhan University*

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Multiphase flow in particle–gas–fluid systems is relevant to many geophysical processes and subsurface engineering applications, such as hydrate production, methane venting, volcanic eruption, etc. Previous researches have investigated the pattern formation in frictional fluid dynamics, viscous fingering instability, wettability alteration, providing the basic understanding of the complex flow mechanisms. Here, we perform laboratory experiments of drainage of liquid–particle mixtures to study morphological patterns and interface stability. We consider both homogeneous and heterogeneous particle distributions. We characterize the flow regime transition from stable displacement to viscous fingering based on morphology and macroscopic metrics, and we compare the onset of fingering with prediction based on the linear stability theory. Compared with homogeneous mixtures, particle clusters and bands in the heterogeneous mixtures evidently promote fingering instability. Furthermore, we find that slow drainage leads to particle compaction bands due to interface ploughing effect. This work provides an improved understanding of the physical mechanism of particle–gas–fluid multiphase flow and is of relevance for practical applications in the subsurface.

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## Flow rate and dissolution rate Impacts on the wormhole formation

**Authors:** Ting Wang<sup>None</sup>; Ran Hu<sup>1</sup>; Zhibing Yang<sup>1</sup>; Yi-Feng Chen<sup>1</sup>

<sup>1</sup> *Wuhan University*

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The dissolution of fractures exhibits various patterns when a reactive fluid was injected into undergrounds. We performed a visual dissolution experiment on NaCl crystals to simulate the coupling of reaction and dissolution in natural environments. Three typical dissolution patterns including face dissolution, wormholes and uniform dissolution were observed. However, the theoretical foundation of transitions of dissolution patterns remains unclear. Here, we proposed a theoretical model to illustrate the transitions of dissolution patterns affected by flow rate and reaction rate. By comparing the length for unsaturated fluids saturates at the radial and transverse direction, the phase diagram predicted by the model shows that wormhole dissolution will dominates when. The phase diagram not only exhibits good agreement with our this and previous experiments, but also is highly consistent with experiments and simulations of existing works. This work extends the classic phase diagram for fracture dissolutions and provide improved insights for dissolving process in subsurface applications.

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MS3 / 74

## Fluid charging and hydrocarbon accumulation in the sweet spot, Ordos Basin, China

**Authors:** Wen Zhao<sup>None</sup> ; Lin Jiang<sup>1</sup> ; Chengzao Jia<sup>1</sup> ; Xiangfang Li<sup>2</sup>

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Although significant progress has been made in the tight gas exploration and development, there is still a limited understanding of the fluid charging and hydrocarbon accumulation in the sweet spot. In this study, a novel method is proposed to generate the stochastically constructed porous media which represents the transition region between tight surrounding sandstone and sweet spot. Based on the constructed porous media, the fluid charging and hydrocarbon accumulation processes of the tight reservoir are simulated by the lattice Boltzmann method (LBM). The numerical simulation results show that, although a piston-like pattern can be observed in field-scale simulation or laboratory experiments, at the micro-scale, due to the inherent heterogeneity of the porous media, the fluid charging pattern tends to be fingering-like. The existence of the transition region between tight surrounding sandstone and sweet spot becomes a water-bearing gas layer or even gas-bearing water layer at the top/bottom of the gas layers (sweet spot). The existence of fractures is favorable for hydrocarbon charging into the reservoir rocks, but not for the hydrocarbon accumulation due to the gas escaping through the fractures. Combined with well logging interpretation results, three typical water bodies (isolated water body, water body at the top, or bottom of the gas layer) are identified from the view of fluid charging and hydrocarbon accumulation.

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## Fluid flow control devices with 3D-graded permeability

**Authors:** David B. Robinson<sup>None</sup> ; Maher Salloum<sup>None</sup> ; Denis Ridzal<sup>None</sup> ; Drew P. Kouri<sup>None</sup>

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Chemical engineering systems often rely on components that involve intimate contact between a fluid and a solid, such as in catalyzed reactive flows, fluid purifiers, and chromatographic separations. To accomplish this, it is often necessary to distribute the fluid from a relatively narrow tube to a broader cross section, to an array of tubes, or into a porous medium that can be modeled by Darcy's Law or similar flow model. Ideally, the flow rates in the tube array or throughout the porous medium are uniform, and the size, weight, and cost of this portion of the system are a small fraction of those of the chemically reactive portion.

Additive manufacturing techniques raise the possibilities that porous media can be fabricated in which the permeability can be arbitrarily specified in three dimensions, and that a broader range of permeabilities can be achieved than by traditional methods used to manufacture porous media.[1] We are using optimization algorithms [2] to design devices that distribute a fluid from a narrow inlet to a broad outlet, where the outlet flow rate is spatially uniform, and device geometry and/or pressure drop are constrained, by spatially varying the permeability in the device. We have considered a Darcy's law model, as well as a modification of the Navier-Stokes equations with a term representing permeability.[3] Numerical models show that designs varying permeability in three or two dimensions can achieve greater uniformity than designs that vary permeability in only one dimension (such as with stacked flow elements).

Meanwhile, we are evaluating methods to fabricate structures with spatially varying porosity on conventional additive manufacturing tools, as a path to build the designed devices for future experimental testing.

Our work is supported by the Laboratory-Directed Research and Development program at Sandia National Laboratories, a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.  
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## Fluid rearrangements during Haine's jumps using time-resolved micro-computed tomography

**Author:** Kim Robert Tekseth<sup>1</sup>

**Co-author:** Dag Werner Breiby<sup>2</sup>

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Multiphase flow in porous media has high societal relevance, for example in geological CO<sub>2</sub> sequestration and gas diffusion in fuel cells. Intensive research over several decades has been conducted on multi-phase flow in two dimensions using setups such as Hele-Shaw cells[1,2]. Advances in X-ray sources and detectors have made time-resolved studies of flow in three-dimensional porous media feasible through computed tomography (CT). Time-resolved CT is usually carried out at synchrotron facilities, because home-laboratory setups have a low photon flux resulting in long exposure times and consequently poor time resolutions. However, by utilizing advanced tomographic reconstruction algorithms exploiting *a priori* information about the sample, one can alleviate the projection sampling requirement, reducing the time-resolution down to tens of seconds, compared to minutes or hours in the case of regular CT scans[3].



Here, we present results from a time-resolved two-phase flow imbibition and drainage experiment using an industrial CT instrument (Nikon) with a custom-made sample stage, giving a spatial resolution better than 10  $\mu\text{m}$  and a time resolution of about 30 s per scan [4]. The porous sample was a sintered glass bead pack of 250-500  $\mu\text{m}$  diameter soda-lime spheres initially filled with a (non-wetting) air phase in a capillary of 2.5 mm inner diameter. The dynamics consisted of first injecting and then withdrawing a 0.5 M KI doped water at a volumetric flow rate of 0.12  $\mu\text{L}/\text{min}$ . The good time-resolution was achieved by acquiring undersampled tomographic datasets and using an iterative algorithm that utilizes both *a priori* sample information and *compressed sensing* techniques to faithfully reconstruct the 3D sample[5]. Specifically, the algorithm exploits that the sintered and inert glass beads were stationary throughout the experiment. The acquisition time was further reduced by placing the syringe pumps on a rotational stage with power being transferred through a slip ring, allowing repeated rotations in one direction (see Fig. 1A).

The results showed a stable displacement process of air by doped water during imbibition, while the drainage process was dominated by fingering, consistent with literature[6,7]. During drainage, we observed slow interfacial fluid curvature changes followed by quick pore-filling events (cf. Fig 1D), consistent with what is known as Haine's jumps[8]. Preliminary results also indicate that these Haine's jumps, with a volume of about 0.05  $\mu\text{L}$ , can be reversible and repeated, by cycling the volumetric flow rate periodically [4].

The combination of the experimental setup and the reconstruction algorithm presented here has the potential to explore a wide range of 3D multi-phase flow phenomena in porous media, in the home-laboratory for challenging and calibrating theoretical models.

#### Acknowledgements

We gratefully acknowledge the Research Council of Norway for financial funding through the FRINATEK project *4D-CT*, project no. 275182, and the Centre of Excellence funding scheme, project no. 262644 (CoE *PoreLab*).

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## Fluid-Fluid Displacement in Mixed-Wet Porous Media

**Authors:** Ashkan Irannezhad<sup>1</sup> ; Bauyrzhan Primkulov<sup>2</sup> ; Ruben Juanes<sup>2</sup> ; Benzhong Zhao<sup>3</sup>

<sup>1</sup> *McMaster University*

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Fluid-fluid displacement in porous media occurs in many natural and engineering processes such as water infiltration into soil, geological carbon dioxide storage, and enhanced oil recovery. It has long been recognized that wettability plays an important role in the displacement process. For instance, the displacement pattern of a viscous ambient fluid by a less viscous invading fluid becomes more compact as the invading fluid becomes more wetting to the porous medium. Thanks to decades of research, we now have a fairly good understanding of fluid-fluid displacement in porous media with uniform wettabilities. In contrast, our knowledge of fluid-fluid displacement in porous media with heterogeneous wettabilities (i.e., mixed-wet) is much less complete, even though mixed-wet conditions are common in many subsurface processes.

Here, we study the impact of mixed-wettability on fluid-fluid displacement in simple porous media. Experimentally, we perform constant-rate displacement of a viscous ambient fluid by a less viscous invading fluid in microfluidic flow cells patterned with vertical posts. We image the system at high resolution, providing simultaneous visualization of both the physics of wetting at the pore scale and the impact of wetting on the macroscopic displacement pattern. By tuning the surface energy of the flow cell locally, we achieve clusters of posts that are distinctly more wetting to the invading fluid compared to the rest of the flow cell. We vary the wettability of the clusters, as well as their size and distribution. We find that they both exert important control over the displacement pattern. Numerically, we simulate the experiments using a novel pore network model (Primkulov et al., 2019). We achieve excellent agreement between the modeling results and the experiments. Our work provides an experimental and numerical platform to systematically investigate fluid-fluid displacement in mixed-wet porous media.

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## Fluid-driven particle transport patterns in fractures

**Author:** Xinwei Hu<sup>1</sup>

**Co-authors:** Zhibing Yang<sup>1</sup> ; Yi-Feng Chen<sup>1</sup>

<sup>1</sup> *Wuhan University*

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It remains challenging to fully understand the granular transport mechanisms in confined geometries like fractured media. Here, by performing massively parallel simulations based on a coupled computational fluid dynamics and discrete element method (CFD-DEM) approach, we systematically investigate the particle transport patterns and mechanisms driven by fluid flow in both smooth and rough fractures. In smooth fractures, depending on the local drag force, the particles can settle or suspend in the fluid, leading to fluid-driven particle transport by creeping or by suspension.

Fluid-induced fingering patterns are observed in the upper layer of settled particles during the sliding. It is shown that the fingering pattern is affected by the flow rate and particle volume fraction. In rough fractures, increasing the standard deviations of the aperture shifts the particle migration from uniform to fingering behavior, which leads to earlier breakthrough and increased particle trapping.

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## Fluid-fluid phase separation in a soft porous medium

**Authors:** Oliver Paulin<sup>1</sup> ; Liam Morrow<sup>1</sup> ; Matthew Hennessy<sup>1</sup> ; Chris MacMinn<sup>1</sup>

<sup>1</sup> *University of Oxford*

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The interactions of two fluids within a porous medium depend strongly on flow conditions, wettability, and the structure of the pore space. At the pore scale, these interactions are characterised by the formation of wetting films that coat solid surfaces and occupy corners and throats, and the formation of non-wetting blobs that occupy larger pore bodies. The invasion of non-wetting blobs into narrow throats is energetically unfavorable, but it can be forced with a sufficiently high pressure gradient. A soft porous medium is one in which the pore structure can deform in response to the flow. The most striking feature of two-fluid-phase flow in a soft porous medium is the tendency of the non-wetting phase to enlarge the pore space by pushing the solid grains apart, to the point of forming macroscopic cavities in the medium. These cavities can be much larger than the pore scale, and they form spontaneously when the energetic benefit of reducing the Laplace pressure exceeds the energetic cost of deforming the solid skeleton. Here, we consider this process through the lens of phase separation, where a non-wetting phase separates (or not) from a fluid-fluid-solid mixture. Informed by the thermodynamics and large-deformation poromechanics of this system, we construct a phase-field model in which two immiscible fluids interact with a poroelastic solid skeleton. Our model captures the competing effects of elasticity, confinement, flow, and fluid-fluid-solid interactions. We then use our model to consider an initial distribution of non-wetting fluid in the pore space that separates into multiple cavities. We identify the key parameters that control phase separation, the conditions that favor the formation of cavities, and the characteristic size of the resulting cavities. We complement this analysis with experimental observations. Our results have implications for a wide variety of natural and industrial systems, such as the nucleation and growth of gas bubbles in lake beds and waste ponds.

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## Fluid-solid interfacial area at different wetting conditions during multiphase in a porous medium

**Authors:** Deepshikha Singh<sup>1</sup> ; Jyoti Phirani<sup>1</sup>

<sup>1</sup> *IIT, Delhi*

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Wettability and wettability alteration plays a vital role in many applications to understand the hydraulic conductivity and quantify many Darcy scale flow parameters during multiphase flow in a porous medium. The wettability influences the fluid-solid and fluid-fluid interfacial areas. Ideally, the fluid-solid interfacial area in a porous medium for a non-wetting fluid can be zero when thin films of the wetting fluid quote the solid surface. Therefore, quantifying the fluid-solid interfacial area can provide a way to measure wettability at Darcy scale. The two-tracer method has been explored to quantify the fluid-solid interfacial area during the multiphase flow through a porous medium for a given wettability. Here we demonstrate the influence of the different wettability on the quantified solid-fluid interfacial area. For this, we use the two-tracer method to investigate the fluid-solid interfacial area's relationship with wettability and saturation. We prepare a proxy porous medium consisting of fractional weight of the hydrophilic (water-wet) and hydrophobic (oil-wet) glass beads in the cylindrical tube's packing. We investigate the consequences of the wettability alteration on the estimated fluid-solid interfacial area during the multiphase flow in a porous medium at various residual saturations. We report our measurements of the fluid-solid interfacial area at different saturations for varying wettability condition.

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## Fluid-structure interactions in a soft-walled Hele-Shaw cell

**Authors:** Callum Cuttle<sup>1</sup> ; Satyajit Pramanik<sup>1</sup> ; Jian Hui Guan<sup>1</sup> ; Chris MacMinn<sup>1</sup>

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The interaction of viscous and interfacial flows with soft materials has recently attracted substantial interest from a variety of different perspectives. Here, we study these interactions in the context of a model problem: Flow in a deformable Hele-Shaw cell, where one wall is rigid and the other is soft. Combining experiments with mathematical modelling, we consider the coupling of flow and deformation as air is injected into a cell initially filled with viscous fluid. We examine how deformation affects the viscous fingering instability and discuss the implications of our results for related physical systems.

We acknowledge financial supports from EPSRC EP/P009751/1 and ERCH2020 805469.

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MS15 / 324

## Flux Regression Performances of Deep Learning in Discrete Fracture Networks

**Authors:** Stefano Berrone<sup>1</sup> ; Francesco Della Santa<sup>2</sup> ; Antonio Mastropietro<sup>2</sup> ; Sandra Pieraccini<sup>None</sup> ; Francesco Vaccarino<sup>2</sup>

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The need of flow and transport characterization in underground fractured media is critical in many engineering applications, like fossil fuel extraction and water resources analysis. However, there is a lack of full knowledge (geometrical and hydrogeological) of these fracture systems and, therefore, statistical representations of the fractured media are given. In this context, we perform flow simulations in underground fractures with Discrete Fracture Network (DFN) models.

The stochastic representation of the fracture systems requires thousands of DFN generations and simulations to characterize the flow in a real fractured medium. For this reason, it is desirable to consider the application of Deep Learning models and use them as alternative model reduction methods to speed up the flow characterization process.

In this work we show the application of a set of Deep Learning models for flux regression in Discrete Fracture Networks, analyzing the regression quality and revealing suitable enhancements of the already existing encouraging results [1].

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## Forced air and water flow in granular media – models and experiments

**Author:** Ilan Ben-Noah<sup>1</sup>

**Co-authors:** Shmulik P. Friedman<sup>2</sup> ; Ido Nitsan<sup>3</sup>

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The physical processes governing advective and diffusive gas and a counter-current, convective water movement in soil are discussed and described using flow models and in situ measurements in controlled environment experiments. We present several coupled-flow models using analytical solutions to describe simplified physical problems and/or numerical models to describe in more detail the coupled, two-phase flow.

In general, air flow in wet soils is governed by three main forces: capillary, viscous, and gravitation (buoyancy). These forces are characterized by the capillary number (Ca), i.e. the ratio between viscosity and capillary forces, the Bond number (Bo) number, i.e. the ratio between gravitational and capillary forces, by the viscosity ratio of the fluids (M), and by the ratio between these dimensionless numbers.

For the case of gas injection into an unsaturated soil, where a “background” capillary pressure, significantly larger than the air entry value prevails (e.g. a phreatic surface located below the flow domain of interest), the macroscopic air flow is expected to follow the continuum approach formulation (Richards equation) for a much larger span of Ca, Bo and M numbers.

Furthermore, in the case of forced two-phase flow, i.e. independent injection of air and water, the water pressure gradient is expected to alter the effect of these  $\square$  numbers on air flow regime and distribution. For example, the role of buoyancy in the vertical water flow depends on the water flux direction (and magnitude), where a downward water flux reduces the effect of buoyancy while an upward water flow increases its effect.

Experiments, describing the effects of water content and forced two-phase flow (gas and water) were conducted in one- (narrow column) and three- (large Plexiglas barrels) dimensional set-up conditions. Measurements of transient and steady-state distributions of O<sub>2</sub> concentration, water and air pressure, and volumetric water content for different tracer gas (N<sub>2</sub> or air) injection rates (on a large span of Ca numbers), cycle duties, cycle periods, and injection depths are used to study several two-phase flow processes and phenomena, e.g., a counter-current flow of immiscible fluids, unsteady density-driven flow, hydrodynamic hysteresis, intrinsic and relative soil's air and water permeability, buoyancy effect, etc.

Interchanging between air (20.9% O<sub>2</sub>) and N<sub>2</sub> (0% O<sub>2</sub>) gas injection enabled us to estimate the relative effect of counter O<sub>2</sub> diffusion from the atmosphere, and in a complementary manner to evaluate the efficiency and effectiveness of forced soil aeration.

Comparing measurements to the prediction of different models is used to evaluate the applicability of different physical assumptions and of the continuum approach for describing air flow. Furthermore, several non-dimensional numbers and optimization parameters were proposed and evaluated using both measurements and models.

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## Free flow over porous media: Heterogeneity and the Beavers-Joseph interface condition

**Authors:** Matthijs de Winter<sup>1</sup> ; Kilian Weishaupt<sup>2</sup> ; Amir Raouf<sup>1</sup> ; Rainer Helmig<sup>2</sup>

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Whether it is river water slowly flowing over a sand bed, water flowing in between activated carbon electrodes in a Blue Energy setup, a gentle breeze of air across partially saturated soil or car fumes

over the catalyst body in the exhaust pipe... the coupling of laminar free flow and parallel flow through porous media (Darcy) can be described by the Beavers-Joseph interface condition. The BJ-interface condition assumes a non-zero slip velocity at the interface between the free flow channel and the porous media. The slip velocity relates the free flow velocity to the Darcy velocity through the permeability of the porous media and a second material parameter, called the Beavers-Joseph coefficient. The latter is based on experimental data.

We investigate the coupling between a free flow channel (Poiseuille flow) and a heterogeneous porous medium. We find that introducing heterogeneity strongly influences the behavior at the interface. A perfect symmetry effectively prohibits mass exchange across the interface, while the non-symmetric porous media promotes mass exchange across the interface.

We will show the simulation results from a large collection of domains with free flow over a heterogeneous porous media and show that the evaluation of the BJ slip velocity may have surprising outcomes due to the exchange of mass across the interface. The mass exchange has also consequences for the efficiency of solute mixing across the interface. Moreover, we will focus in on the fluid behavior at pore scale levels and discuss our attempts to up-scaling our findings to Darcy length scales.

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## From the non-linear Darcy law for immiscible two-phase flow in porous media to constitutive equations for each fluid species

**Authors:** Subhadeep Roy<sup>1</sup> ; Håkon Pedersen<sup>1</sup> ; Santanu Sinha<sup>2</sup> ; Alex Hansen<sup>3</sup>

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There is growing evidence that the flow velocity  $\vec{v}_p$  of an immiscible fluid mixture flowing in a porous medium depends on the local pressure gradient to a power in the range 1.5 to 2 when capillary and viscous forces compete [1]. The relative permeability equations relate the flow velocity of each immiscible fluid species,  $\vec{v}_w$  and  $\vec{v}_n$ , to a gradient in the corresponding pressure field. These equations allow the mapping  $(\vec{v}_w, \vec{v}_n) \rightarrow \vec{v}_p$ . However, the opposite mapping,  $\vec{v}_p \rightarrow (\vec{v}_w, \vec{v}_n)$  is not unique. Hence, attempts at generalizing the relative permeability equations to account for the non-linear behavior of  $\vec{v}_p$  cannot use  $\vec{v}_p$  as a starting point. Hansen et al. [2] have defined a co-moving velocity  $\vec{v}_m$  which is related to but not equal to the velocity difference between the two fluid species and provided a transformation  $(\vec{v}_p, \vec{v}_m) \rightarrow (\vec{v}_w, \vec{v}_n)$ , making it possible relate the non-linear behavior of  $\vec{v}_p$  to non-linearities in the behavior of  $\vec{v}_w$  and  $\vec{v}_n$ . We use a dynamic network model [3] and relative permeability data from the literature to explore this mapping and what it means.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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MS7 / 302

## GMsFEM for Reduced Model of Darcy Flow in Fractured Porous Media

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In This work, we combine Generalized Multiscale Finite Element Method (GMsFEM) with a reduced model based on Discrete Fracture Model (DFM) to resolve the difficulties of simulating fluid flow in fractured porous media while efficiently and accurately reduce the computational complexity resulting from resolving the fine scale effects of the fractures. The geometrical structure of the fractures is discretely resolved within the model using DFM. The advantage of using GMs- FEM is to represent the fracture effects on a coarse grid via multiscale basis functions constructed using local spectral problem. Solving local problem leads to consider small scale information in each coarse grid. On another hand, the multiscale basis functions, generated following GMsFEM framework, are parameter independent and constructed once in what we call it offline stage. These basis functions can be re-used for solving the problem for any input parameter when it is needed. Combining GMsFEM and DFM has been introduced in other works assuming continuous pressure across the fractures interface. This continuity is obtained when the fractures are much more permeable than that in the matrix domain. In this work, we consider a general case for the permeability in both fracture and matrix domain using the reduced model presented in [3]. The proposed reduction technique has significant impact on enabling engineers and scientist to efficiently, accurately and inexpensively solve the large and complex system resulting from modeling flow in fractured porous media.

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## Gas shale swelling and shrinkage characterized by controlled suction experiments



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Gas shales are partially water saturated with their pore space simultaneously filled with brine and liquid and/or gas hydrocarbons. Changes in water saturation can cause swelling or shrinkage, which is of significant importance to natural gas production from unconventional shale reservoirs and sample handling in the laboratory [1]. During hydraulic fracturing, a substantial amount of injected water-based fluid is believed to imbibe into the shale matrix, driven by the high suction gradient between the well and the shale. Such imbibition has been evidenced in the field by large fluid loss during flowback operations and reproduced by many laboratory spontaneous imbibition tests [2], [3]. Also highlighted in recent research is that increasing water saturation can not only result in swelling [4] but also alter elastic and strength properties [5]. However, little is known about how suction and water saturation can be related to the resulting volumetric deformation in gas shales. Here we show our progress in characterizing the swelling and shrinkage of gas shales as stress-strain behavior. We found, in our controlled suction experiments on an organic-rich shale, that the volumetric strain induced by suction variations is a strong function of imposed suction and water saturation. The non-linear hysteretic relationship between the two was expressed by water retention curves. We discuss possible expressions for the average pore pressure and effective stress. We anticipate our results to be a starting point for a more sophisticated stress-strain framework with a proper definition of effective stress for partially saturated gas shales.

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## Gas water two phase flow in fractured-porous carbonates

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The recoverable natural gas in carbonate reservoirs account for 45% of the total gas reserves. However, the physical heterogeneity of carbonate reservoirs is strong, and the fractures play a strong role in flow controlling. Therefore, gas-water two-phase flow in fractured carbonates is the key to

hydrodynamic modeling of gas reservoir development with bottom and edge water. Here, using in situ X-ray microtomography, we provide the observational evidences of dynamic trapped gas and residual water distribution in a fractured carbonate. Finally the characteristics of gas–water flow during the gas flooding and water flooding in a fractured carbonate rock were described. We found that the gas preferentially entered into large pores and connected fractures due to the large gas flow resistance in micro fractures. The gas began to enter into micro fractures until the gas flooding pressure was increased to 1 MPa. Inversely, water preferentially entered into micro fractures during water flooding, because gas-water flow is mainly controlled by capillary force at low flooding rate (0.01 mL/min). As the water film thickened, water flowed along the fracture wall in the form of connected phase, while disconnected bubbles or gas columns flowed in the middle of the fracture. Furthermore, we concluded three types of trapped gas, which are trapped gas formed at dead ends and blind corners, trapped gas formed by Jamin effect and snap-off. We also studied the size distribution of individual trapped clusters in the pore space. The gas cluster volume  $V$  plotted against cluster surface area  $A$  also correlated with a power-law correlation  $A \propto V^p$ , and  $p$  was always  $\approx 0.75$ . The gas-cluster-size distributions were measured and followed a power-law correlation  $N \propto V^{-\tau}$ , where  $N$  is the frequency with which clusters of volume  $V$  are counted, and decays exponents  $\tau$  is 0.22.

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## Gas-liquid phase separation in a soft porous medium

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Various biological and chemical processes can lead to the nucleation and growth of gas bubbles within the pore space of an otherwise liquid-saturated granular medium, such as in lake beds and waste ponds. The gas is typically non-wetting and, as the bubbles approach the pore size, it is energetically costly for them to invade narrow pore throats. If the solid skeleton is sufficiently soft, it is favourable for the bubbles to displace the solid grains and form macroscopic cavities. Here, we consider this process through the lens of phase separation, where thermomechanics govern the separation of a gas phase from a gas-liquid-solid mixture. We construct a phase-field model informed by large-deformation poromechanics, in which two immiscible fluids interact with a poroelastic solid skeleton. Our model captures the competing effects of elasticity and gas-liquid-solid interactions. As a model problem, we consider an initial distribution of gas in the pore space that separates into multiple gas cavities. We identify the key parameters that control phase separation, the conditions that favour the formation of gas cavities, and the characteristic size of the resulting gas cavities.

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## Generalized coupling conditions for arbitrary flows to the fluid-porous interface

**Authors:** Elissa Eggenweiler<sup>1</sup> ; Marco Discacciati<sup>2</sup> ; Iryna Rybak<sup>1</sup>

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Coupled systems containing a free-flow region and a porous-medium domain appear in many technical applications, biological and environmental settings, e.g., industrial filtration, cell proliferation, surface water/groundwater flow. The interaction between the free flow and the porous-medium flow is dominated by the interface driven processes. Thus, for accurate modeling and numerical simulation of such coupled flow problems the correct choice of coupling conditions at the fluid-porous interface is crucial.

We use the Stokes equations to describe the fluid flow in the free-flow region and Darcy's law in the porous-medium domain. In order to couple the two different systems of equations, the conservation of mass, the balance of normal forces and the Beavers-Joseph coupling condition on the tangential velocity component, which was proposed for flows parallel to the fluid-porous interface, are typically applied. However, this set of interface conditions is not suitable for arbitrary flows to the fluid-porous interface [1].

In this talk, we present new, generalized coupling conditions for the Stokes-Darcy problem, which are valid for arbitrary flow directions to the fluid-porous interface [2]. These conditions are derived rigorously using the theory of homogenization with two-scale asymptotic expansions and boundary layers. Under the assumptions on parallel flow to the porous bed, the developed generalized interface conditions reduce to the ones proposed by Jäger and Mikelić [3]. All coefficients appearing in the new coupling conditions are computed numerically based on the pore geometry of the coupled system and are independent of the macroscopic flow direction. The generalized conditions are validated using pore-scale resolved simulations [2]. The developed coupling conditions are compared to the classical ones highlighting the advantages of the new conditions. The well-posedness of the Stokes-Darcy problem with new interface conditions is studied.

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## Generating unrepresented geological realizations using Generative Adversarial Networks

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In this work, we investigate the capacity of Generative Adversarial Networks (GANs) in generating unrepresented patterns in a geological dataset. The new unrepresented patterns in the training dataset are assumed to belong to the same original data distribution. Specifically, we design a conditional GANs model in a supervised training of GANs, to interpolate geological properties between the training classes. The presented study includes an investigation of various training settings and model architectures. In addition, we devised new conditioning routines, for an improved generation of the missing samples. The presented numerical experiments on images representing binary channels showed good geological consistency as well as strong correlation with the target conditions.

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## Generation of Virtual Nonwoven Structures and Simulation Studies of Compression Behavior and Flow Permeability

**Authors:** Sarah Staub<sup>1</sup> ; Sridhar Ranganathan<sup>2</sup> ; Stefan Rief<sup>1</sup> ; Konrad Steiner<sup>1</sup>

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Nonwovens are highly porous media, typically used in industrial applications to transport and absorb fluids and/or to insulate against heat and noise. Moreover, they should be mechanically stable, especially under high compression. In the current talk, Kimberly-Clark and Fraunhofer ITWM present their joint work on modelling the mechanical compression behavior of thin nonwoven and the impact on the resulting material properties.

The focus lies on thin nonwoven structures consisting of different fiber types. We generate virtual geometry models that possess the essential properties of a given reference medium. These properties comprise the caliper, the basis weight, fiber orientations and fiber composition. Furthermore, based on  $\mu$ CT images, the pore size distribution of the reference structure is determined. It turns out that the first virtual models have all desired properties except for the pore size distribution. The real medium shows larger pores. Hence, we established a two-step generation algorithm. First, a packing of spheres is created whose size distribution resembles the larger pores. In a second step, a non-overlapping fiber generator enters the desired fibers and, finally, deletes the spheres. By doing so, it is possible to validate the virtual medium against measured flow permeabilities.

Kimberly-Clark and Fraunhofer ITWM agreed on geometrical variations of the virtual reference medium to study the effects of changes in fiber diameters and fiber orientations. Moreover, based on this virtual models simulation studies of the mechanical compression behavior are performed. Of special interest is the impact of the number of bonding points between the fibers. In contrast to the number of fibers contained in the simulation box, the number of connection points between the fibers is not unique. Therefore, we present a procedure to compare the number of bond points in different structures.

The mechanical simulations are performed by ITW's simulation tool FeelMath, which is also commercially available as the ElastoDict module in the software package GeoDict. This solver employs the Lippmann-Schwinger equations for elasticity in the Fourier space. Due to the voxel-based approach, large structures containing several thousands of highly resolved fibers and bonds are simulated. A further advantage of this method compared to Finite-Element approaches is the applicability to highly porous structures without the need of a mesh generation.

This effective approach allows for the numerical study of many virtual realizations, which are necessary to capture the variance of fiber networks with similar characteristics. In addition to the simulation of the mechanical effective stiffness of the nonwovens, the effective permeability is simulated and compared to experimental results.

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## Geometry evolution and fracture alteration controlled by spatial mineral heterogeneity during CO<sub>2</sub> sequestration – A reactive transport study

**Authors:** Mohammad Nooraiepour<sup>1</sup> ; Hossein Fazeli<sup>2</sup> ; Mohammad Masoudi<sup>3</sup> ; Helge Hellevang<sup>4</sup>

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Geological CO<sub>2</sub> storage and CCS have a crucial role in reducing CO<sub>2</sub> emission and therefore mitigating climate change. One of the prerequisites for selecting CO<sub>2</sub> storage sites is a low permeability caprock preventing potential CO<sub>2</sub> leakage and migration from the storage reservoir. The presence of fractures in the caprock can adversely affect the sealing capacity of caprocks. Chemical interactions between CO<sub>2</sub>, brine, and caprock-forming minerals can cause fracture evolution, which results in changes in the transmissivity of fractures within the sealing layers. One factor that can affect the chemically induced fracture alterations is mineral heterogeneity in the caprock. In the present work, we investigate the effect of mineral heterogeneity on fracture geometry evolution when CO<sub>2</sub>-rich brine flows through a single fracture scribed on different carbonate-rich caprock samples. The rock samples have different carbonate contents and different levels of mineral heterogeneities. They can represent carbonate-rich caprocks such as some intervals of the Upper Jurassic (Kimmeridgian) Draupne shales, the caprock for Smeaheia CO<sub>2</sub> storage in Norway. An HPHT geomaterial microfluidic experimental setup is used to monitor the evolution of the fractures. Results indicate that the homogeneous caprock samples, i.e., the samples mainly composed of calcite, show a uniform fracture wall dissolution while fracture wall roughness increases for heterogeneous samples. The effluent chemistry analyses show that the sample-scale calcite dissolution rate decreases over time, which can be due to the mass transfer limitations in the boundary layer near the fracture wall (for the homogeneous sample) or the altered layer formed around the fracture (for the heterogeneous samples). Microfluidic experiments were also done for one carbonate-rich fine-grained shale sample, which showed dissolution of calcite with no macroscopic fracture alteration during the ten-day experiment. This indicates that in shale samples where the carbonate minerals, mainly calcite, are armored with other slow reacting minerals such as clays, the rate of fracture geometry evolution will be prolonged, which might be a positive point for the caprock integrity. However, the confirmed fluid-rock geochemical interactions within the shaly sample in a short time frame call for further investigations on the consequent impacts on caprock samples' geomechanical-hydrological properties for more extended periods relevant for subsurface CO<sub>2</sub> storage. The microfluidic experiments are

also used to validate a reactive transport model. The model will then be utilized to study changes in transport properties of different samples during experiments. The LBM-based model outputs, such as porosity-permeability relationships, can inform reactive models at larger scales to develop a better predictive numerical simulator for processes involved in CO<sub>2</sub> storage projects.

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## Geostatistical Inversion in Geologic CO<sub>2</sub> Sequestration Using a Variational Autoencoder

**Authors:** Bailian Chen<sup>1</sup>; Dylan Harp<sup>1</sup>; Daniel O'Malley<sup>None</sup>; Rajesh Pawar<sup>2</sup>

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Geostatistical inversion problems in geologic CO<sub>2</sub> sequestration (GCS) often involve matching observational data using a physical model that takes a large number of parameters. It is known that solving an inversion problem in a high-dimensional space with complex structure is usually a very time consuming process. In this work, a dimensionality reduction technique, variational autoencoder (VAE), was proposed to efficiently invert storage reservoir parameter fields (e.g., permeability) with the aim of improving predictions of important metrics such as pressure and CO<sub>2</sub> saturation maps. A gradient-based optimization algorithm, L-BFGS, is utilized to minimize the observational and predictive data mismatch function. A VAE is trained to map to a low-dimensional set of latent variables with a simple structure to the high-dimensional parameter space (i.e., original space) that has a complex structure. The required optimization process to fit model to observational data will then be performed on a low dimensional latent space, making the gradient-based optimization (i.e., L-BFGS) more computationally efficient. The feasibility and efficiency of the proposed approach for GCS inverse analysis were demonstrated with a 3D synthetic case. A preliminary result is shown in the figure. (Figure caption: Predictions of CO<sub>2</sub> saturation plume at the end of post-injection period based on the updated models under different monitoring durations (1 yr, 3 yrs, etc.))

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## Glass Micromodels Study of Emulsified Polymer Gel System for Conformance Control Applications

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Different techniques were used for water shut off and conformance control in the mature oil fields whose sole purpose is to cut the water production and sweep the oil towards the producing wells. Many different types of gel systems were developed for the conformance control but all of them have the risk associated with them. It is common for the gel systems to not only block the water producing zone, but they also block the oil producing zone. To solve this problem an invert emulsion system with polyacrylamide (polymer) and polyethyleneimine (crosslinker) was developed. The emulsion system breaks into oil phase and gelant phase at high temperature of 105 °C. The oil phase will provide a path for the oil to flow towards the producing well whereas the gel will prevent the water from flowing towards the production well. To understand this behaviour properly, microfluidic experiments were conducted in this work.

To understand the emulsion separation and conformance control behaviour of developed invert emulsion system, the glass micromodels were used. The developed emulsion was injected into the micromodel and heated at 105 °C for emulsion separation and gelation.

After the gelation in the glass micromodels, the injection of water and oil was carried out and the behaviour of water and oil flow was recorded using the microscopic camera. The video graphic analysis presented a unique way in which the developed emulsion systems prevents the water production but allows the oil to flow.

This work for the first time presented the mechanisms which were used by the emulsion system to provide efficient conformance control, the use of micromodel allowed to visually see how the emulsion system allows the oil flow but restricts the water production.

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## **Global implicit solver for multiphase multicomponent flow in porous media with multiple gas components and general reactions**

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In order to study the efficacy of mineral trapping scenarios for CO<sub>2</sub> storage behaviour in deep layers, demanding highly nonlinear coupled diffusion-advection-reaction partial differential equations (PDEs) have to be solved.

The chemistry includes both general kinetic and equilibrium reactions.

Realistic scenarios further ask to simulate the inflow of various gases into the deep layers.

We solve the multiphase multicomponent flow equations by means of a fully globally implicit PDE reduction method (PDERM) for the case of an arbitrary number of species in gaseous phase which are injected into a deep layer.

The Finite Element discretized / Finite Volume stabilized equations are split into a local and a global system coupled by the resolution function and evaluated with the aid of a nested semismooth Newton solver.

Our methods are implemented within the free open source software M++.

We present realistic scenarios of gas injection into deep layers and study the mineral trapping effects

of the storage technique.

Finally, the PDERM reduction method can be applied not only to CO<sub>2</sub> storage processes, but also to e.g. oil recovery and nuclear waste storage.

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M.M. Knodel, S. Krättele, P. Knabner: Global implicit solver for multiphase multicomponent flow in porous media with multiple gas phases and general reactions. In: Finite Volumes for Complex Applications IX - Volume I and Volume II; FVCA 9, Bergen, Norway, June 15-19, 2020. Editors: R. Klöfkorn, E. Keilegavlen, A.F. Radu, J. Fuhrmann. Springer Proceedings in Mathematics and Statistics.

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## **Global random walk solvers for flow and multi-component reactive transport in heterogeneous porous media**

**Authors:** Nicolae Suci<sup>1</sup> ; Florin Adrian Radu<sup>2</sup>

<sup>1</sup> *University of Erlangen-Nuremberg*

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Flow and multi-component reactive transport in unsaturated/saturated porous media are modeled by ensembles of computational particles moving on regular lattices according to specific random walk rules. The occupation number of the lattice sites is updated with a global random walk (GRW) procedure which simulates the evolution of the ensemble with computational costs comparable to those for a single random walk simulation in sequential procedures. To cope with the nonlinearity and the degeneracy of the Richards equation the GRW flow solver uses linearization techniques similar to the *L*-scheme developed in finite element/volume approaches. Reactive transport schemes, coupled with the flow solver via numerical solutions for saturation and water flux, are implemented in splitting procedures. Diffusion-advection steps are solved by GRW algorithms using either biased or unbiased random walk rules. Since the number of particles in GRW simulations can be as large as the number of molecules involved in chemical reactions, one avoids the cumbersome problem of rescaling particle densities to approximate concentrations. Reaction steps are therefore formulated in terms of concentrations, as in deterministic approaches. The numerical convergence of the new reactive scheme is demonstrated by comparison with analytical solutions of a model problem for nonlinear bi-molecular reactions. Coupled flow-reactive transport problems of contaminant biodegradation based on a Monod type model are further solved and the influence of flow nonlinearity/degeneracy and of the spatial heterogeneity of the medium is investigated numerically.

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## Global sensitivity analysis of a low permeability media gas flow model with multiple transport mechanisms

**Authors:** Leonardo Sandoval<sup>1</sup> ; Monica Riva<sup>1</sup> ; Ivo Colombo<sup>2</sup> ; Alberto Guadagnini<sup>1</sup>

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Methane is recognized as a potential energy source in the transition to carbon free energies. Appropriate modeling approaches to quantify methane migration in low permeability geomaterials can assist the appraisal of the feasibility of a methane recovery project. Wu et al. (2016) proposed a model enabling one to estimate the total mass flow rate of the gas as the sum of key processes, including (i) a surface diffusion and two weighted bulk diffusion components, (ii) slip flow, and (iii) Knudsen diffusion. In its isothermal form and taking pressure gradient as boundary condition, the model relies on 10 parameters. These are typically estimated through laboratory-scale experiments. Considering the mechanisms involved, such experiments are costly, time demanding, and their results are prone to uncertainty. The latter is also related to the intrinsic difficulties linked to replicating operational field conditions at the laboratory scale as well as to the desired transferability of results to heterogeneous field scale settings. Due to our still incomplete knowledge of the key mechanisms driving gas movement in low permeability geomaterials and the complexities associated with the estimation of model parameters, model outputs should be carefully analyzed considering all possible sources of uncertainty. In this sense, sensitivity analysis approaches may be used to enhance the quality of parameter estimation workflows, upon focusing efforts on parameters with the highest influence to target model outputs. We rely on two typical global sensitivity analysis approaches (i.e., Variance-based Sobol approach and Morris method) to analyze the behavior of the aforementioned gas migration model targeting low permeability media. Because of the complexity of the physical processes represented in the model and the typical frequency distributions of pore size in caprocks, the sensitivity analysis is performed in two differing settings, each corresponding to a given range of variability of characteristic pore sizes. When considering porous systems with pore size ranging between 2 and 100 nanometers, results based on Sobol indices identify (in decreasing order of importance) pore radius, porosity, pore pressure, and tortuosity as the parameters whose uncertainty significantly imprints model output uncertainty. Similar results are obtained through the analysis of the Morris indices, these identifying the pore radius parameter as the one with the highest contribution to non-linear (or interaction) effects on the model output. For tighter porous media (i.e., with pore size comprised between 2 and 10 nanometers), the Sobol indices analyses identify (in decreasing order of importance) pore pressure, porosity, blockage/migration ratio of adsorbed molecules, and pore radius as the most influential model parameters. The role of the blockage/migration ratio of adsorbed molecules suggests that surface diffusion is a dominant gas transport mechanism in these scenarios. The Morris approach identifies the same parameters as important, albeit in a different order of importance.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Wu, K., Chen, Z., Li, X., Guo, C., Wei, M., 2016. A model for multiple transport mechanisms through nanopores of shale gas reservoirs with real gas effect-adsorption-mechanic coupling. *International Journal of Heat and Mass Transfer* 93, 408-426. doi: 10.1016/j.ijheatmasstransfer.2015.10.003 **Acceptance of Terms and Conditions:**

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## Graded viscosity banks on the rear end of the polymer slug

**Authors:** Fedor Bakharev<sup>1</sup> ; Aleksandr Enin<sup>1</sup> ; Sergey Tikhomirov<sup>1</sup> ; Konstantin Kalinin<sup>1</sup> ; Yulia Petrova<sup>1</sup>

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One of the problems in EOR methods is the instability that occurs on the interface between two fluids with high viscosity contrast. The usage of viscous polymer agent can partially solve the problem by making the water-oil front stable. However the subsequent displacement of polymer by water produce a lot of long thin “water fingers” on the rear end of the polymer slug. The breakthrough of the polymer slug reduces the oil recovery factor. In the talk we will discuss how to calculate the size of polymer slug and consider the technology of graded viscosity banks (GVB) which helps to reduce the amount of polymer mass without loss of it’s effectiveness.

GVB technology was proposed by Claridge and consists in injecting several subsequent polymer slugs of decreasing concentrations. As viscosity ratio reduces, the instabilities start to grow slowly and one can inject less amount of polymer with the same positive effect on oil recovery.

The main assumption of GVB technology is the linear growth of the front and rear ends of the mixing zone. There are a lot of numerical works that confirm linear behavior of fingers at intermediate times, but unfortunately no rigorous results exist up to now. However it is possible to get pessimistic estimates on velocities of the mixing zone by analyzing the mathematical model of the miscible displacement (the so-called Peaceman model) under transverse flow equilibrium assumptions. Unlike the well-known Koval and Todd-Longstaff models, these estimates take into account not only the viscosity ratio, but the whole viscosity curve. In the talk we will give an overview of the existing models and present our results in this direction.

From practical point of view a natural question arises: “How many slugs should one inject?” To answer this question we calculate the amount of saved polymer for  $n$  slugs and prove a theorem that there exists a limiting injection profile as number of slugs tends to infinity. This gives an upper bound on the possible amount of saved polymer. Analyzing the result for different viscosity curves and finger velocity models we conclude that for many practical situations it is enough to inject 2-5 slugs.

We verify the GVB technology with our numerical experiments in DuMuX.

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## Gradient discretization of two-phase flows coupled with mechanical deformation in fractured porous media

**Authors:** Francesco Bonaldi<sup>1</sup> ; Konstantin Brenner<sup>2</sup> ; Jérôme Droniou<sup>3</sup> ; Roland Masson<sup>4</sup> ; Antoine Pateau<sup>5</sup> ; Laurent Trenty<sup>5</sup>

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In this talk, we consider a two-phase Darcy flow in a fractured and deformable porous medium for which the fractures are described as a network of planar surfaces leading to so-called hybrid-dimensional models. Fractures are assumed open and filled by the fluids, and small deformations with a linear elastic constitutive law are considered in the matrix. At matrix-fracture interfaces, phase pressures can be continuous or discontinuous, corresponding to two different models. Unlike single-phase flow, discontinuous pressure models for two-phase flows provide a better accuracy than continuous pressure models even for highly permeable fractures. This is due to the fact that fractures fully filled by one phase can act as barriers for the other phase, resulting in a pressure discontinuity at the matrix fracture interface. The model is discretized using the gradient discretization method, which covers a large class of conforming and non-conforming schemes. This framework allows for a generic convergence analysis of the coupled model using a combination of discrete functional tools. Numerical solutions provided by the continuous and discontinuous pressure models are compared on gas injection and suction test cases using a Two-Point Flux Approximation (TPFA) finite volume scheme for the flows and  $\mathbb{P}_2$  finite elements for the mechanics.

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## Graphene oxide nanoparticles for aquifer remediation: transport experiments and reactivity batch tests.

**Authors:** Ali Beryani<sup>1</sup> ; Carlo Bianco<sup>1</sup> ; Tiziana Tosco<sup>1</sup> ; Mohammad Reza Alavi-Moghaddam<sup>2</sup> ; Rajandrea Sethi<sup>1</sup>

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Graphene oxide nanoparticles (GONPs) proved effective in the adsorption of a broad set of environmentally relevant contaminants, such as organic aromatic compounds, heavy metals, dye molecules, pharmaceuticals (Iqbal and Abdala, 2013; Zhou et al., 2016). Moreover, thanks to their small size, GONPs could be injected in the subsurface for the in-situ treatment of contaminated aquifer systems. A key step in the development of such remediation technology is the study of the injectability and mobility of GONP suspensions in porous media, as well as of their reactivity against contaminants.

In this study, three GONP sources were considered (two commercial, one synthesized in the laboratory). A systematic study was carried out exploring the influence of GO type, size (300 – 1200 nm), concentration (10 – 50 mg/L), and sand size (coarse to fine) on its transport in sand-packed columns (15 cm long, 1.6 cm diameter) at a Darcy velocity of  $8.11 \times 10^{-5}$  m/s. The main aims were (i) to evaluate which parameters mostly influence GONP transport, (ii) to identify the main mechanisms of GONP interaction with the porous medium, (iii) to verify if the advection-dispersion-deposition

model, developed for round-shaped colloids, is quantitatively reliable also for GONPs, characterized by a clearly different structure. Particles were stably dispersed in water and showed a good mobility in the porous medium in all conditions: after injection of 5 pore volumes and flushing, the highest recovery was around 90%, the lowest around 30% (only for large particles in fine sand). This suggested that injection and distribution in groundwater should not be challenging. The particle size was by far the most impacting parameter, even if sand size and particle concentration were also relevant. The numerical model MNMs 2021 (Bianco et al., 2016) ([www.polito.it/groundwater/software](http://www.polito.it/groundwater/software)) proved adequate to describe GONP transport in the porous medium, both from a qualitative and quantitative point of view: transport was correctly described by a two-site deposition (reversible blocking and irreversible straining) (Beryani et al., 2020).

As a second part of this study, the capability of GONPs to remove organic contaminants was characterized through batch adsorption tests. Methylene blue (MB) was opted as a model molecule representative of these contaminants of concern, which could be absorbed by GONPs in aquatic environments. MB is a common aromatic, water soluble, cationic dye which has been reported as a major pollutant of water resources because of its carcinogenicity and other health adverse effects on aquatic organisms and humans. Additionally, MB removal processes can be representative of other contaminants removal procedures since electrostatic interactions,  $\pi$ - $\pi$  stacking and hydrogen bonds are the most effective phenomena governing all adsorption processes.

The adsorption experiments demonstrated that GO is highly effective in the rapid adsorption of MB, hereby chosen as a model molecule representative of cationic contaminants. However, it shows a maximum capacity to attract MB on its surface. In this study, the estimated adsorption capacity of GOs was observed at a mass ratio of MB/GO equal to 1.

#### Time Block Preference:

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MS1 / 577

## Gravitational instabilities in a 2D porous medium for carbon dioxide sequestration

**Authors:** Jayabrata Dhar<sup>1</sup> ; Shabina Ashraf<sup>1</sup> ; François Nadal<sup>2</sup> ; Patrice Meunier<sup>3</sup> ; Yves Méheust<sup>4</sup>

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With an ever-increasing global warming scenario, geological sequestration stands as an effective mean to trap gases such as carbon dioxide (CO<sub>2</sub>) towards long-term storage. The subsurface trapping

mechanisms occurring upon injection of supercritical carbon dioxide (sCO<sub>2</sub>) are structural, residual, solubility, and mineral trapping [1-3]. Among them, success of solubility trapping dictates the efficient long-term storage capability of geological sequestration [4-6]. During solubility trapping, the less dense sCO<sub>2</sub> positioned under the cap rock begins to dissolve in the aquifer water/brine, thereby creating an interface of aqueous mixture containing dissolved carbon dioxide over the aquifer [7,8]. That mixture is denser than the brine medium beneath it. This unstable stratification develops into a gravitational instability. A natural convection of dissolved CO<sub>2</sub> ensues within the brine and allows for more resident liquid to be subsequently available for dissolution of the sCO<sub>2</sub> into it [1,9,10]. The dynamics of CO<sub>2</sub> dissolution and gravitational fingering, as described above, has been mostly studied using Darcy scale simulations [6,8]. However, the applicability of the Darcy-scale approximation to the coupled convection and solute transport process at play in solubility trapping is not obvious. We present here an experimental study in a granular porous medium, aiming at investigating the range of the validity of the Darcy scale approximation and observe under which conditions, and to which extent, the numerical predictions for the time scales of CO<sub>2</sub> storage, based on such approximations, under- or over-predict the experimental results.

Our analogue experiment is based on refractive index matching of the fluid (a solution of Triton X-100, water and zinc chloride) to the solid grains (spherical PMMA beads, which renders the 3D porous medium transparent. The density contrast between the heavier and lighter (miscible) liquid phases comes from the amount of ZnCl<sub>2</sub> added, while the heavier fluid also contains a dye (at a small concentration) to allow tracking the interface evolution and fingering structures. Varying the density of the heavier fluid and the PMMA bead size allows controlling the Rayleigh (Ra) and Darcy (Da) numbers. Measurements are performed in quasi-two-dimensional conditions. The data consists of images recorded at a regular time interval and post-processed using MATLAB. Darcy scale numerical simulations of the experimental configuration are performed using the software COMSOL Multiphysics. The experimental and numerical results are compared in terms of the mixing length, finger velocity and finger number density. We observe that the presence of the granular porous medium strongly impacts the gravitational instability dynamics (as compared to the simulated dynamics), and this all the more as the characteristic number  $Ra\sqrt{Da}$  is larger. For  $Ra\sqrt{Da} > 1$  the simulation results largely under-predicts the experimental data. More importantly, this under-prediction doesn't cancel out entirely when the Darcy regime is valid ( $Ra\sqrt{Da} < 0.1$ ), i.e., when the typical scale of convection fingers is larger than the pore size. This finding may suggest that the coupling between gravity-actuated Stokes flow and solute transport cannot be simply upscaled to the Darcy scale using coupled Darcy's law and a dispersive solute transport equation.

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## Gravity-driven instability in fracture flows with miscible fluids of different densities

**Authors:** Hongfan Cao<sup>None</sup> ; Seonkyoo Yoon<sup>None</sup> ; Zhenyu Xu<sup>1</sup> ; Laura Pyrak-Nolte<sup>1</sup> ; Etienne Bresciani<sup>None</sup> ; Peter Kang<sup>2</sup>

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Many important subsurface processes and applications, such as geologic carbon sequestration, enhanced geothermal system, and magma flow in dykes, involve flows of variable-density fluids in geologic fractures. Understanding the role of variable-density flow on transport, mixing, and geochemical reactions is essential for the prediction, design, and operation of the subsurface activities. In reality, vertical fractures are common, and flow and transport in vertical or inclined fractures will determine the integrity of caprocks. However, the effects of density contrasts on flow and mixing in vertical fractures have rarely been studied.

In this study, we combine visual laboratory experiments and direct three-dimensional (3D) numerical simulations to study the effects of fracture inclination angle (orientation relative to gravity), flow inertia, and density contrasts between fluids on the spatiotemporal distribution of miscible fluids in a fracture. Two miscible fluids with different densities are injected through two inlets at the bottom of the fracture and flowed out from the outlet at the top of the fracture. The density contrast between two injection fluids results in the lighter fluid being confined to a narrow path, which we term “runlet”, and the instability of this runlet is observed in both visual lab experiments and 3D numerical simulations. We investigate the underlying mechanisms triggering the instability in variable-density fracture flows by systematically conducting numerical simulations for various combinations of flow rates, density contrasts, and fracture inclination angles. We first identify critical stagnation points that control the instability of the runlet through streamline and flow topology analysis. We then elucidate the effects of fluid stretching and mixing on the evolution of critical stagnation points by analyzing the spatiotemporal evolution of stretching and mixing measures. Our results show that the runlet is formed by the complex interplay between the density contrast, inertia effects, and mixing, and the runlet instability is controlled by 3D vortices.

The experimental work supported by the former Center for Nanoscale Controls on Geologic CO<sub>2</sub> (NCGC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award # DE-AC02-05CH11231

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MS9 / 383

## Growth and upscaling of viscous fingers in immiscible two-phase flow

**Authors:** Santanu Sinha<sup>1</sup> ; Hursanay Fyhn<sup>2</sup> ; Subhadeep Roy<sup>3</sup> ; Alex Hansen<sup>2</sup>

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A less viscous fluid invading into a more viscous immiscible fluid produces fingering patterns due to instabilities at the interfaces between them. In the space between two closely spaced parallel plates, the fingers appear to be smooth as there is essentially only one interface separating the fluids. In case of a porous medium, e.g. by filling the space between the plates with fixed glass beads, the fingers show fractal structures where many microscopic fluid-fluid interfaces exist. These patterns are fractal in nature and characterized by different fractal dimensions depending on whether they are dominated by viscous or capillary forces [1].

In the large-scale continuum limit where the pores are vanishingly small compared to the dimensions of the porous medium, the relative density of invading fluid in the fractal patterns approaches zero. Rather, it is the structures giving rise to non-zero saturation which will dominate. The local saturation is the proper quantity to characterize the fingers in this limit.

We now ask the following question: Is it possible to use the fractal structures on the pore scale to infer the saturation distribution in the continuum limit? We follow the experimental work of Løvoll et al. [1] and Toussaint et al. [2], using an averaging technique to map out a probability distribution for the position of the fingers. That is, each point is given a probability density for being part of a viscous finger. This creates a density profile and we conjecture that this density profile reproduces the saturation profile in the continuum limit. This conjecture is built upon the work of Arnéodo et al. [3] that demonstrated that averaging over DLA patterns reproduces the smooth fingers that Saffman-Taylor found analytically.

We perform our study with dynamical pore-network modeling [4] and analytical derivations [5], and compare them with experimental observations.

### Time Block Preference:

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## Growth of gas-filled penny-shaped cracks in decompressed hydrogels

**Authors:** Yansheng Zhang<sup>1</sup> ; Merlin Aragon Etzold<sup>1</sup> ; Adrien Lefauve<sup>2</sup>

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We report experiments in which hydrogels equilibrated with carbon dioxide at elevated pressure experience sudden decompression. The hydrogels remain stable until disturbed by a small impact, which initiates the formation of penny-shaped cracks within the hydrogel. The main radius of these oblate ellipsoids grows linearly in time with a growth rate of the order of 1 cm/minute.

Our quantitative model assumes the growth kinetics of the crack to be controlled by gas diffusion from the bulk of the hydrogel to the crack boundaries. Crack propagation continuously creates fresh crack surface whose high gas concentration supports continuous crack growth. The model confirms the observed linear growth of the main crack radius and predicts the growth rate with high accuracy from the material properties.

This work might be of interest as catastrophic mechanism of tissue damage for decompression sickness and to study material properties via cavitation rheology.

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## **HYDRUS and analytical modeling of seepage in porous banks of commingled ephemeral streams having triangular flash-flood hydrographs: emergence and extinction of an “ephemeral” unconfined aquifer**

**Authors:** Anvar Kacimov<sup>None</sup>; Jiri Šimůnek<sup>1</sup>

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Perched aquifers (PA) are important sources of groundwater in arid/semiarid climates where surface water resources are irregular (see, e.g., Intermittent..., 2017). PAs as hydrostratigraphic units are commonly conceived as being created/maintained by vertical infiltration from a vadose zone above aquifer's phreatic surface and vanished due to a) vertical percolation, which descends into a subjacent vadose zone under aquifer's thin low-permeable bed, and b) vertical ascending seepage flow driven by evapotranspiration. In our work, we study “ephemeral” aquifers, whose advent and disappearance are controlled by prevalently horizontal fluxes, one into a vadose zone and another into a conterminous ephemeral stream. Initial-boundary value problems to the Richards 2-D equation, 1-D Boussinesq equation, and 2-D Laplace equation are solved in models of saturated-unsaturated and purely saturated flows. At  $t < 0$ , both the stream and adjacent bank (wedge-shaped in a vertical cross-section) are dry. At  $t > 0$ , a flash flood takes place. Wadi's water first imbibes into the bank and later exfiltrates back through the slope, which is made of two discharging segments: a seepage face and ponded interface between stream's water and the aquifer (Fig. 1a).

The process is controlled by a specified wadi hydrograph. We focus on the case of a constant rate drawup-drawdown regime, i.e., the wadi stage rises-drops linearly with time. Analytical (Barenblatt et al., 1984) and numerical (HYDRUS-2D, Šimůnek et al., 2016) solutions compare well. Dynamics of bank's phreatic surface (conjugated with the wadi water level), transient fluxes, pore-water storage in the bank, loci of the tips of the wetting fronts (propagating along a bedrock of an emerged “ephemeral” unconfined aquifer), pore pressure isobars (in particular, the position of the crest of an evolving groundwater mound), piezometric contours, vector fields of Darcian velocity, isotachs, and streamlines in the three models are studied. Fig. 1b illustrates a snapshot of HYDRUS pore pressure heads for the drawup phase. A rapid drawup of the wadi level and slow post-flash-flood drawdown generate an intricate topology of groundwater and soil moisture motion, viz. the three phases of



expansion-slumping-*evanescence* (E-S-E). For example, in the slumping phase, a stagnation point emerges on the bedrock at a certain time and flow bifurcates into one halve, which keeps moving to the right in Fig. 1a, and another discharges through the slope. The mound may or may not be intercepted by a dormant (not-pumping) well in the riparian zone. The well is tracked by HYDRUS observational nodes. Depending on the phase of aquifer's evolution ("yes"-*yes*"-*no*" in the example of Fig.1b), the distance between the well and wadi, screen's depth, and hydraulic properties of soil, the phreatic surface either intersects the well or not. If yes, a well operator can start abstracting groundwater. Implications for intelligent interception of short-lived groundwater pockets by on-bank farms and for groundwater banking in MAR projects are discussed. Another application of our HYDRUS and analytical models is in the ecohydrology of riparian phreatophytes (e.g., the Christ-thorn trees, Al-Maktoumi et al., 2020). Ecotones of this wild vegetation are aligned with wadis' and can serve as bioindicators of the post-flash-flood extension of ephemeral aquifers in Fig. 1a.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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MS21 / 188

## Heat and mass transfer in a shear-thinning fluid through porous media

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Heat and mass transfer in non-Newtonian fluids through porous materials have wide applications in nature and engineering. Compared to non-Newtonian fluid flow in porous materials, solute and heat transport in porous materials have been less investigated. Specially, effect of heterogeneity of porous structure on flow and transport and upscaling the bulk fluid properties to the porous media averaged properties are not yet well understood.

To address these gaps in understanding, we proposed a GPU-parallelized pore-network model to simulate the flow and dynamic transport of non-Newtonian fluids in 3D unstructured networks with millions of pores at the centimetre level. The modified Meter model was used to properly model the relation between viscosity and shear stress of the non-Newtonian fluid under varying temperatures. We first validated the algorithm by comparing the thermal front from simulation results against the proposed analytical solution. Then both Newtonian and non-Newtonian fluids were studied in the spatially uncorrelated and correlated networks at varying injecting flow rates. The proposed modelling framework provides the possibility to control the injection rate as a function of porous media properties and fluids rheology. Additionally, effect of spatial heterogeneity and

dynamic conditions on thermal fingering and upscaling transport properties will be presented in this work.

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MS15 / 489

## Heterogeneity Evaluation of Microstructures in a Sandstone Reservoir Using Micro-CT Imagery

**Author:** Lingyun Kong<sup>1</sup>

**Co-authors:** Bethany Kurz<sup>2</sup>; Shane Butler<sup>2</sup>; Matthew Burton-Kelly<sup>2</sup>; Cesar Barajas-Olalde<sup>2</sup>; Blaise Mibeck<sup>2</sup>; Xue Yu<sup>3</sup>

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Heterogeneity of microstructures in clastic rocks is relevant to a wealth of subsurface properties (e.g., porosity, permeability, fracture orientations) and, yet, is challenging to effectively characterize because of the stochastic distribution of grain deposition, diagenesis, and texture deformation. At the pore to core scale, heterogeneity lies in the spatial variation of pore throat networks and complicates the fluid flow mechanisms associated with those networks. Therefore, it is essential to precisely comprehend the heterogeneity at the fine scale, which further facilitates understanding at a broader scale (well to basin). In this study, micro-CT (computed tomography) images of samples from a conventional sandstone reservoir were collected. The heterogeneity was evaluated in terms of the microstructure variation (pore size distribution, pore shape distribution, and porosity variation) in three dimensions spatially and the associated petrophysical property changes derived from images. Firstly, the representative elementary volume (REV) was determined by extracting the subvolumes at increasing sizes inside of CT image data sets. REV was set to 100 voxels (20.7  $\mu\text{m}/\text{voxel}$ ) to capture the representative area to assess heterogeneity. An ImageJ Macro algorithm was coded to automatically resample the subvolume from a 100-voxel size to a 600-voxel size for a cube-shaped region of interest. A machine learning-assisted thresholding method was developed to segment the grain matrix and pore structures. Further, microstructure variation was calculated by processing subvolumes, with the permeability derived by adopting the Kozeny–Carman equation. The statistics from the above parameters demonstrate both the size effect and spatial effect of the region of interest existing in the sandstone reservoir. Moreover, the fractal dimension, a mathematical parameter indicating the self-similarity and complexity of a subject, was utilized to quantify the heterogeneity of microstructures at increasing subvolume sizes, where the same trend was revealed as fractal dimension increasing from 2.6 to 2.95. The database obtained via quantitative evaluation of the microstructure variation within the sandstone samples provides for machine learning-informed image analysis and is an essential step toward heterogeneity characterization across various scales.

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MS1 / 555

## Heterogeneity effects on the Solubility-trapping during CO<sub>2</sub> Geological Sequestration

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In the CO<sub>2</sub> sequestration process, the solubility-trapping mechanism is one of the key mechanisms, which contributes to the safe eradication of injected supercritical CO<sub>2</sub> (ScCO<sub>2</sub>). When ScCO<sub>2</sub> is injected into the reservoir domain, it will start migrating upwards due to its low density as compared to reservoir water. During this migration, some amount of CO<sub>2</sub> will be dissolved into the reservoir water. This process of CO<sub>2</sub> dissolving in the reservoir water and getting trapped in the reservoir domain is known as Solubility-trapping. The dissolution of CO<sub>2</sub> in the reservoir domain can also occur due to the solubility fingering phenomenon. This solubility fingering phenomenon takes place due to the density differences between the CO<sub>2</sub> dissolved water and connate reservoir water. Further, it will cause instability in the domain, which activates the diffusive convection process, which will increase the solubility-trapping efficiency gradually [1].

The objective of this paper is to conduct a study on solubility-trapping mechanisms during the CO<sub>2</sub> sequestration process. The solubility-trapping mechanism has a greater influence on the mineral-trapping mechanism, where the harmful CO<sub>2</sub> can be permanently eliminated by mineral dissolution and precipitation reactions [2]. In this research, an effort is made to study the influences of petrophysical properties, geomorphological structures, and other CO<sub>2</sub> sequestration parameters on the solubility-trapping mechanism over a long geological time scale. The reactive transport modelling technique is used to perform this numerical analysis. It has the ability to predict the geochemical reactions in both spatial and temporal directions along with the fluid flow [3]. In the current numerical analysis, necessary assumptions are made so that only the solubility reactions are considered by neglecting the mineral reaction.

Firstly, the evidence of solubility-trapping due to the instability created by density differences in the reservoir domain is evaluated. Then the initiation of density-driven convective mixing is evaluated with the help of the Rayleigh-Darcy number for an observable domain over a geological time scale. Secondly, the parametric analysis is carried out by analyzing the solubility-trapping percentage at different injection points with a fixed injection rate so that the optimal injection point for CO<sub>2</sub> sequestration is evaluated. Then the influences of petrophysical properties and geomorphological structure on the solubility-trapping mechanism are studied by modelling individual synthetic domains.

Further, the analysis is carried out to study the trapping efficiency, storage capacity, and structural integrity. These simulation analyses are carried out based on the cumulative aqueous CO<sub>2</sub> concentrations, average reservoir pressure, and reservoir temperature. The outcome of these results provide insights into the selection of the suitable range of petrophysical properties and optimal injection points for the safe and efficient implementation of CO<sub>2</sub> sequestration.

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## Heterogeneous Wettability in Porous Catalyst Layers of PEM Fuel Cells: Modeling-based Analysis and Design

**Authors:** Wolfgang Olbrich<sup>1</sup> ; Thomas Kadyk<sup>2</sup> ; Ulrich Sauter<sup>3</sup> ; Michael Eikerling<sup>2</sup>

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Polymer electrolyte membrane (PEM) fuel cells are expected to play an integral role as low-emission energy converters in a future energy economy. Although technological maturity of these cells has been demonstrated, the challenge remains to achieve high power performance at drastically reduced platinum loading. So far, the attempts to reduce the platinum loading have been thwarted by severe voltage losses. A possible origin of these losses is the water flooding of porous gas-transport media. The optimal water balance is of particular importance for the operation of the cathode catalyst layer (CCL), wherein liquid water is needed for efficient proton transport and high activity of the oxygen reduction reaction [1], whereas excessive water accumulation in pores (i.e., flooding) would block the porous pathways needed for the gaseous supply of oxygen. An optimal design of porous electrode media PEM fuel cells should thus account for heterogeneous wettability effects in them.

Conventional CCLs possess an agglomerate structure with a bimodal porous network morphology [2]. Primary pores (1-10 nm diameter) exist in the carbon support, which has platinum particles (1-5 nm diameter) attached to its surface. Secondary pores (10 – 50 nm diameter) form the space between Pt-loaded carbon. An ionomer-subphase is dispersed in this structure, forming a thin, skin-like layer that partially covers the surface of Pt/C particles or their agglomerates.

The CCL exhibits a highly heterogeneous wetting behavior. Various models [3, 4] account for the impact of the mixed wettability, parametrizing contact angles and fractions of hydrophilic/hydrophobic parts independently to match experimental data. We propose a novel approach that harnesses the correlations between the wetting behavior and the structure and composition of the layer. The main distinction is made between ionomer-penetrated and ionomer-free pores. The impact of the Pt particle density on the support is also explicitly considered. Moreover, a peculiar ionomer inversion effect that had been seen in previous experimental results plays a crucial role: where ionomer covers the Pt/C surface, previously hydrophilic surfaces turn hydrophobic [5]. Consequently, we developed a set of descriptors, including a statistical density function for wetting properties. Our analysis of the relations between structure, composition, wettability and performance supports the following hypothesis: lowering the Pt loading via reducing the Pt:C ratio evokes hydrophilic wetting behavior in secondary pores, leaving the CCL highly susceptible for flooding. Based on this finding, we derive design strategies to match low-Pt-loading with flooding-resistant wetting behavior. The results of this work are embedded in larger framework of a comprehensive, structure-based model to link CCL recipe and material choices with performance.

**Time Block Preference:**

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MS16 / 340

## High Speed-Laser Speckle imaging to unravel pico-liter droplets substrate interactions

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In printing industry research effort are currently focused on understanding evaporation and imbibition process of pico-liter droplets [1, 2, 3]. In addition to new commercial inks and formulations, new machines and technologies are evolving. Understanding phenomena such as evaporation and imbibition of pico-liter droplets into porous thin substrates, is therefore crucial in printing industry to achieve a higher printing quality and print speed.

In this contest we present an instrument which can print on-demand pico-liter volume droplets of ink onto substrates, and then immediately record the evolution of the resulting dynamics when these two materials interact. The technique, High Speed Laser Speckle Imaging (HS-LSI), evolution of standard LSI [4], has been developed to monitor nanometer displacement of the drying and imbibing ink droplet at high frame rate, up to 20kHz, given the short timescales of these interactions. We show the results obtained using two different inks printed on three substrates. Inks are home-made with two latices with different glass transition temperature ( $T_g$ ), namely  $-16^\circ\text{C}$  and  $37^\circ\text{C}$ . The substrates are glass filters, (PTFE) sheets and Teslin paper. The former material has been chosen following as it is unable to swell while the pore size and surface properties mimicking common printing paper. A substrate with no swelling ensures that the recorded dynamics are associated with the movement of the tested ink only. The second, PTFE, is hydrophobic: neither water nor water-containing substances can wet it. Teslin paper is a single-layer waterproof synthetic printing medium

In this talk, we will give one example of HS-LSI's usage for unraveling some dynamic printing features on each substrate which cannot be observed using other techniques.

A complete physio-chemical description of the printing, imbibement, and swelling processes associated with commercial ink jet printing are currently under investigation using this HS-LSI instrument

**Time Block Preference:**

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## High-order ADE solution for the fluid diffusion equation and application in coupled hydro-mechanical simulation

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To improve the stability and efficiency of explicit techniques, one proposed method is to use an unconditionally stable alternating direction explicit (ADE) scheme. However, the standard ADE scheme is only moderately accurate and restricted to uniform grids. This paper develops a novel high-order ADE scheme capable of solving the fluid diffusion equation applicable for non-uniform grids. The new scheme is derived by performing a fourth-order finite difference approximation to the spatial derivatives of the diffusion equation in non-uniform grid. The implicit Crank-Nicolson technique is then applied to the resulting approximation, and the subsequent equation is split into two alternating direction sweeps, giving rise to a new high-order ADE scheme. Because the new scheme can be potentially applied in coupled hydro-mechanical (H-M) simulation, the pore pressure solutions from the new scheme are then sequentially coupled with an existing geomechanical simulator in the computer program FLAC. This coupling procedure is called the sequentially-explicit coupling technique based on the fourth-order ADE scheme (SEA-4). Verifications of well-known consolidation problems showed that the new ADE scheme and SEA-4 can reduce computer runtime by 46–75% to that of FLAC's basic scheme. At the same time, the techniques still maintained average percentage error of 1.6–3.5% for pore pressure and 0.2–1.5% for displacement solutions and were still accurate under typical grid non-uniformities. This result suggests that the new high-order ADE scheme can provide an efficient explicit technique for solving the flow equation of a coupled H-M problem, which will be beneficial for large-scale and long-term H-M problems in geoen지니어ing.

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## Higher-Order Finite Element Multiphase Multicomponent Reactive Transport Model for Unstructured and Fractured Grids

**Author:** Mengnan Li<sup>1</sup>

**Co-authors:** Derrick James<sup>1</sup> ; Joachim Moortgat<sup>1</sup>

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We present a higher-order finite element (FE) reactive transport model for unstructured and fractured grids. We use an advanced research simulator (Osures) for flow and transport in subsurface fractured porous media, which models the convection, gravity, mechanical dispersion, Fickian diffusion, Nernst-Planck (electrochemical) diffusion, and capillarity as driving forces. Fluid flow is modeled with the Mixed Hybrid FE method, which provides smooth velocity fields even in highly heterogeneous formations with discrete fractures. Multicomponent species transport is updated with a Discontinuous Galerkin (DG) FE method, which offers strict local mass conservation and low numerical dispersion. The Cubic Plus Association (CPA) equation of state is adopted to compute thermodynamic properties of all fluid phases. CPA considers the self-association of polar molecules and polar-induced cross-association. To incorporate the broadest range of reactions (equilibrium and kinetic, aqueous and rock-fluid, electrokinetics etc.), we leverage the PHREEQC geochemistry engine, which has been widely used for (ground)water / hydrogeology applications and thoroughly validated against a wide array of experimental data. PHREEQC provides interfaces, such as PhreeqcRM, which supports implementation as a geochemistry module within any flow and transport simulation framework. We integrate the PhreeqcRM interface and flow simulator Osures in a sequential iterative operator splitting scheme and utilize OpenMP to enable parallel computations for the pressure solver, phase-splits, DG transport updates, geochemistry, and more. This state-of-the-art higher-order FE reactive transport model is capable of simulating geochemical reactions in the aqueous phase (e.g. cation exchange, electrochemical migration), the interdependence of soluble gas components (e.g., carbon dioxide and light hydrocarbons such as methane) and aqueous-rock geochemistry. It allows for any type of unstructured grids, can incorporate discrete fractures, has low numerical dispersion, and can therefore provide more accurate simulation results on relatively coarse grids and low computational cost. The application domains range from lab to field scales and allow highly heterogeneous and fractured rocks.

Model validations are performed to demonstrate the accuracy and robustness of this model for single-phase and two-phase multicomponent subsurface flow. Scaling analyses are presented to quantify the computational efficiency. Reactive transport problems with increasing levels of complexity are investigated, including the effect of dissolved chemical species on CO<sub>2</sub> solubilities, competitive dissolution/exsolution between CO<sub>2</sub> and light hydrocarbons, and CO<sub>2</sub> injection in a field-scale domain with highly heterogeneous formation properties and discrete fractures [2].

#### **Acknowledgments**

The project was supported in part by the US Department of Energy (DOE) Office of Fossil Energy funding to Oak Ridge National Laboratory (ORNL) under project FEAA-045. ORNL is managed by UT-Battelle for the US DOE under Contract DE-AC05-00OR22725. Acknowledgment is also made to the Donors of the American Chemical Society Petroleum Research Fund for partial support of this research.

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## Hindered thermally driven migration of a drop on a chemically patterned wall

**Authors:** Guangpu Zhu<sup>1</sup> ; Greta Tryggvason<sup>2</sup> ; Jun Yao<sup>1</sup>

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A freely suspended drop in a thermal gradient migrates to the hot side since surface tension is usually a decreasing function of temperature. If the drop is attached to a surface with a temperature gradient, the motion is more complicated. The drop either moves to the hot side or cold side, depending on the contact angle and the viscosity ratio. If the surface is patterned, the wettability, or the contact angle, is different for different patches and here we show, using numerical simulations of two-dimensional flows, that a drop can be brought to a stop at the boundary of two patches, even if the drop moves in the same direction on either patch. Two quantities are defined to judge whether the patterned surface can hinder the thermally driven migration of a droplet, namely, defect strength and minimum defect strength. The patterned surface can hinder the droplet migration only when the defect strength is larger than the minimum defect strength. The minimum defect strength increases with the Marangoni number but decreases with the viscosity ratio. Thus, migration of a droplet is easily hindered for low Marangoni numbers and low droplet viscosity, and these results are summarized in a phase diagram.

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## Homogenization approach to the upscaling of a reactive flow through particulate filters with wall integrated catalyst

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Catalytic membranes can degrade gaseous pollutants to clean gas via a catalytic reaction to achieve green emissions. A catalytic membrane is a three scale porous medium. Membranes used in catalytic filters usually have thickness centimeters or millimeters, and consist of active (washcoat) particles, inert material and microscale, micron size, pores. The washcoat particles are porous material with nanoscale pores. The catalytic reactions are heterogeneous (surface reactions) and they occur on the surface of the nanopores. Obviously, simulations at fully resolved pore scale are not feasible, and upscaling techniques have to be applied. It is known that the same microscale problem can be upscaled to different macroscale equations depending on the characteristic numbers. In this paper we study the homogenization of reactive flow in the presence of strong absorption in the washcoat particles. Two reactive transport regimes are studied, in both the reaction dominates over the convection and the diffusion. Peclet's number in the first one is of order 1, and in the second one it is proportional to the ratio of the thickness of the catalytic membrane and the characteristic length of the microscale pores. Two different upscaled equations are obtained,



respectively. Direct numerical simulation at microscale is used to validate these derived macroscale equations.

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MS3 / 101

## Homogenization of Flow in Porous Media with Isolated Embedded Fractures

**Author:** Patrick Jenny<sup>1</sup>

<sup>1</sup> *ETH Zürich, Switzerland*

**Corresponding Author:** [jenny@ifd.mavt.ethz.ch](mailto:jenny@ifd.mavt.ethz.ch)

A model for homogenized flow in porous media with large inhomogeneities is presented. Classical homogenization relies on representative elementary volumes (REV) large enough that asymptotic macroscopic parameters, e.g. effective permeabilities, can be employed to describe the expected or mean behavior. In this way, Darcy's law, which describes the relationship between macroscopic pressure gradient and volumetric flow rate, was derived. In the presence of large features, however, the required REV size may reach the same order as the geometric reference scale of the problem, and thus effective permeabilities obtained from classical homogenization studies may be unsuited. This is in particular the case for reservoirs with isolated, highly conductive fractures. To see this, consider flow from left to right through a block of finite size. If the latter is small enough, such that some fractures are connected to both left and right boundaries, then the resulting flow will be larger for the same average pressure gradient than through a wider block. In this paper, a new sub-REV continuum model to describe this pre-asymptotic flow behavior is presented. The model relies on a nonlocal multi-media description based on coupled integral-differential equations. The only empirical information required for calibration is the effective permeability of an infinitely large domain, e.g. as obtained from classical homogenization. With a series of numerical studies and comparison with Monte Carlo reference data it is demonstrated that the devised sub-REV model accurately captures mean flow rates and pressure profiles for arbitrary domain sizes.

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MS24 / 259

## Homogenization of the linearized ionic transport equations in random porous media

**Author:** Andrey Piatnitski<sup>1</sup>

**Co-author:** Andro Mikelic

<sup>1</sup> *The Arctic University of Norway, UiT, campus Narvik*

**Corresponding Authors:** apiatnitski@gmail.com, andro.mikelic@univ-lyon1.fr

The talk will focus on rigorous homogenization results for a system of partial differential equations describing the transport of a N-component electrolyte in a dilute Newtonian solvent through a rigid random disperse porous medium. We will consider the nonlinear Poisson-Boltzmann equation in a random medium, describe the stochastic homogenization procedure and formulate the convergence results. Then we will show that the two-scale homogenized system is well-posed. In addition, after separating scales, we will justify that the effective tensor satisfies the so-called Onsager properties, that is this tensor is symmetric and positive definite. This shows in particular that the Onsager theory applies to random disperse porous media.

Previously, similar results were obtained for periodic porous media in (G. Allaire, A. Mikelic, A. Piatnitski, *J. Math. Phys.* 51 (2010)).

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**Poster + / 336**

## **Homogenization of two-phase flow in porous media: A diffuse interface approach explaining capillary pressure-saturation hysteresis**

**Authors:** Stefan Metzger<sup>1</sup> ; Peter Knabner<sup>2</sup>

<sup>1</sup> *FAU Erlangen-Nürnberg*

<sup>2</sup> *FAU Erlangen-Nürnberg*

**Corresponding Authors:** knabner@math.fau.de, stefan.metzger@fau.de

Classical models for two-phase flow in porous media are based on a capillary pressure-saturation relationship. Based on the assumption of thermodynamical equilibrium, this relationship is commonly written as  $P^n - P^w = P^c(S^w)$ , where  $P^w$  and  $P^n$  denote the fluid pressures of the wetting and non-wetting fluid phases, and  $P^c$  is the capillary pressure which depends only on the saturation  $S^w$  of the wetting fluid. Prominent examples for this relation for water/gas systems are the parametrizations by Brooks and Corey and by van Genuchten.

However, it is also known for a long time that this approach has some shortcomings (cf. [Hassanizadeh, Gray, *Adv. Water Res.*, 1993] and the references therein). For example, there is hysteresis in  $P^c-S^w$  curves obtained for drainage and imbibition. This non-uniqueness is due to the absence of a specific description of the interfacial area (cf. [Joekar-Niasar, Hassanizadeh, *Int. J. of Multiphase Flow*, 2011] and the references therein).

In this talk we will present a novel upscaling approach for two-phase flow in porous media. We start from a thermodynamically consistent instationary Navier-Stokes-Cahn-Hilliard model describing the evolution of the two-phase flow on the pore scale and identify the relevant time scales. Separating the different scales in the upscaling process allows us derive local fast scale equations describing the microscale dynamics, which are responsible e.g. for hysteresis effects, and global slow scale equations which can be simplified to a generalized macroscopic Darcy law.

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MS25 / 399

## How Harry Vereecken's work contributes to reach the 2030 global sustainable development goals.

**Authors:** Marnik Vanclooster<sup>1</sup>; Sebastien Petit<sup>2</sup>; Mathias Tidjani<sup>1</sup>; Pierre Tovihoudji<sup>3</sup>; Pierre Akponikpe<sup>3</sup>

<sup>1</sup> *Earth and Life Institute, Université catholique de Louvain*

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**Corresponding Authors:** pierretovihoudji@yahoo.fr, mathias.tidjani@student.uclouvain.be, akponikpe@yahoo.com, marnik.vanclooster@uclouvain.be, sebastien.petit@uclouvain.be

For more than 35 years, Harry Vereecken developed vadose science research, aiming primarily to improve the understanding and prediction of water and contaminant transport processes, supporting sustainable soil and water management. This research is key in the current sustainable development agenda, where multiple objectives are directly related to good and healthy status of soil and water systems. In this contribution, examples are given showing how combined methodologies based on pedotransfer functions, hydrogeophysics and modeling of the soil-water-crop continuum are implemented to generate information supporting sustainable soil and water management strategies. A first example deals with the evaluation of the impact of agricultural policies on groundwater quality in Belgium. In this example, long term groundwater pressures with nitrate on deep unconfined groundwater systems are simulated, allowing to evaluate the reaction time of the system for adapted agricultural policies. These policies were designed to reduce nitrate pressures on groundwater systems from the agricultural sector. In this study, the Belgian soil map, the Belgian geological map, soil physical analysis, Harry's pedotransfer functions, and the WAVE model were used to perform the simulation study. The WAVE model (Vanclooster et al., 1996) was a revision of the SWATNIT model, developed earlier by Harry and co-workers in 1991 (Vereecken et al., 1991). A second example deals with the increase of food security in Benin. Benin inland valleys are currently underexploited and present unique opportunities to increase food production. Yet, the exploitation of these inland valleys requires a better understanding of the hydraulic behavior of these inland valley systems. In this example, it is shown how a combined approach, based on classical soil physical sampling, pedotransfer functions, and remote sensing is used to assess the infiltration characteristics of an experimental inland valley, supporting the design of an appropriate hydrological model of Benin inland valley systems. In both examples, approaches and methods inspired by Harry's works were used.

### References

Vereecken H., M. Swerts and M. Vanclooster, 1991. Description of the SWATNIT model. In : Soil and Groundwater Research Report II, Nitrate in soils. Commission of the European Communities, DGXII, 4th Environmental Research Programme: 262-266.

Vanclooster M., P. Viaene, K. Christiaens and S. Ducheyne, 1996. WAVE: a mathematical model for simulating water and agrochemicals in the soil and vadose environment. Reference and user's manual (release 2.1), Institute for Land and Water Management, Katholieke Universiteit Leuven, Leuven, Belgium

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Time Block C (18:00-21:00 CET) **References:**

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**Invited & Keynote Speakers / 794****How do plants transport water under negative pressure?****Author:** Steven Jansen<sup>1</sup><sup>1</sup> *Ulm University***Corresponding Author:** steven.jansen@uni-ulm.de

A longstanding question in biology is how plants are able to transport water under negative pressure without continuously developing large gas bubbles in their transport system, which would reduce sap transport from roots to leaves. This process, which is known to be driven by transpiration at the leaf level, is highly puzzling because the water transported is saturated with gas and includes insoluble, amphiphilic lipids with a potent surface activity. Yet, plants seem to be able to perform this process seemingly effortlessly on a daily basis.

In this talk, we will discuss the importance of mesoporous cell walls between neighbouring conduits, and their functional significance as safety valves. The 200 to 1,000 nm thick porous cell walls, which have an estimated porosity of 80%, and ca. 20 nm wide pore constrictions, are shown to produce surfactant coated nanobubbles by the local surface tension of lipids at gas-liquid interfaces. In an interdisciplinary approach, an overview of experimental evidence will be presented, together with porous cell wall models, and simulations of multiphase interactions between gas, surfactants, water, and solid substances. These efforts contribute not only to our understanding of the mechanisms of plant water transport, but will also enable us to develop evaporation-driven transport devices that do not rely on fossil fuels. Moreover, understanding hydraulic failure in plants has implications for global water conservation, and how plants will deal with increased levels of drought at many places worldwide.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:****Acceptance of Terms and Conditions:**Click here to agree **Newsletter:****Student Poster Award:****Poster + / 19****How does the power law dependency of flow rate on pressure gradient when viscous and capillary forces compete, scale with system size?****Authors:** Subhadeep Roy<sup>1</sup> ; Santanu Sinha<sup>2</sup> ; Alex Hansen<sup>3</sup><sup>1</sup> *PoreLab*<sup>2</sup> *Beijing Computational Science Research Center, 10 East Xibeiwang Road, Haidian District, Beijing 100193, China.*<sup>3</sup> *NTNU***Corresponding Authors:** alex.hansen@ntnu.no, subhadeep.roy@ntnu.no, santanu.sinha@ntnu.no

When two immiscible fluids flow in a porous media at rates where the capillary and viscous forces compete, there is growing experimental, numerical and theoretical evidence that the flow rate depends on the pressure gradient minus a threshold pressure to a power between 1.5 to 2 [1]. At higher flow rates, where viscous forces dominate, the flow rate becomes proportional to the pressure gradient.

Imagine a porous medium of linear size  $L$ . There is a pressure difference  $\Delta P$  between inlet and outlet, resulting in a flow rate

$Q$  across it. When the viscous and capillary forces compete, we have  $Q \sim (\Delta P - P_t)^\beta$  where  $P_t$  is the threshold pressure. When the viscous forces dominate, we have  $Q \sim \Delta P$ . We pose here two questions: (1) what happens to the threshold pressure  $P_t$  as  $L \rightarrow \infty$  and (2) what happens to the pressure difference

$\Delta P_c$  at which  $Q$  goes from non-linear to linear dependence on  $\Delta P$ ?

Based on analytical result from the capillary fiber bundle model and numerical evidence from a dynamic network simulator [2], we demonstrate that  $P_t \rightarrow 0$  and  $\Delta P_c \rightarrow 0$  in this limit,  $L \rightarrow \infty$ .

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

[1] Tallakstad, K. T., Knudsen, H. A., Ramstad, T., Løvoll, G., Måløy, K. J., Toussaint, R., and Flekkøy, E. G., *Phys. Rev. Lett.*, 102, 074502 (2009); Tallakstad, K. T., Løvoll, G., Knudsen, H. A., Ramstad, T., Flekkøy, E. G., and Måløy, K. J., *Phys. Rev. E*, 80, 036308 (2009); Sinha, S. and Hansen, A., *EPL*, 99, 44004 (2012); Roy, S., Hansen, A. and Sinha, S., *Front. Phys.* 7, 92 (2020). Aursjø, O., Erpelding, M., Tallakstad, K. T., Flekkøy, E. G., Hansen, A., and Måløy, K. J., *Front. Phys.* 2, 63 (2014); Sinha, S., Bender, A.T., Danczyk, M., Keepseagle, K., Prather, C.A., Bray, J.M., Thrane, L.W., Seymour, J.D., Codd, S.L. and Hansen, A., *Transport Por. Media*, 119, 77 (2017); Gao, Y., Lin, Q., Bijeljic, B. and Blunt, M. J., *Water Resources Research*, 53, 10274 (2017); Gao, Y., Lin, Q., Bijeljic, B. and Blunt, M. J., *Phys. Rev. Fluids*, 5, 013801 (2020); Zhang, Y., Bijeljic, B., Gao, Y., Lin, Q. and Blunt, M. J., *eartharXiv*, <https://doi.org/10.31223/osf.io/2rxbn> (2020).

[2] Roy, S., Sinha, S. and Hansen, A., arXiv:1912.05248. **Acceptance of Terms and Conditions:**

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MS22 / 32

## How does the structure of a gas diffusion layer control the performance of fuel cells

**Authors:** Daniel Niblett<sup>None</sup> ; Adrian Mularczyk<sup>1</sup> ; Jens Eller<sup>1</sup> ; Stuart Holmes<sup>2</sup> ; Vahid J Niasar<sup>None</sup>

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Gas diffusion layer (GDL) is one of the components in PEM fuel cells. The performance of PEM fuel cells is affected by the transport loss which is due to the complex two-phase flow of gas-liquid in the GDL and gas channel. In this presentation, we show how ordered structures for GDLs can improve the performance of fuel cells.

Water management within fuel cell porous transport layers is a key challenge for improving performance. When liquid water accumulates at a high current density, the oxygen diffusion resistance is increased. Additionally, we present the effect of GDL, microporous layer (MPL) and gas channel (GC) structure on the liquid water percolation and detachment in the channel.

Dynamic two-phase flow simulations have been performed using OpenFOAM® with the Volume of Fluid (VoF) method to evaluate the water distribution in 2D and 3D ordered and disordered porous media. This study highlights the importance of pore morphology in improving two-phase flow dynamics. The simulation approach was compared to x-ray micro-computed tomography data of water injected into a GDL with detachment in the channel, which showed a high level of agreement. The effects of GDL pore morphology, defects in the MPL, and interaction between GDL and GC on the water dynamics in the system have been studied.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Daniel Niblett, Adrian Mularczyk, Vahid Niasar, Jens Eller, Stuart Holmes, Two-phase flow dynamics in a gas diffusion layer - gas channel - microporous layer system, Journal of Power Sources, Volume 471, 2020,228427 **Acceptance of Terms and Conditions:**

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**Poster + / 474**

## How heterogeneous distributions of wettability affects infiltration into soil

**Author:** Jonas Bentz<sup>1</sup>

**Co-authors:** Eva Kröner<sup>2</sup> ; Ravi Patel<sup>3</sup>

<sup>1</sup> *Universität Koblenz-Landau*

<sup>2</sup> *Forschungszentrum Jülich*

<sup>3</sup> *Karlsruher Institut für Technologie*

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A central component of the rhizosphere is root mucilage, a hydrogel exuded by plants that dramatically alters chemical and physical properties of the soil. It is characterized by its large water holding capacity and is hydrophilic or hydrophobic depending on its hydration status: when swollen, mucilage is hydrophilic but becomes hydrophobic when dry, forming local hydrophobic spots on the surface of soil particles. The morphology of these hydrophobic regions formed by dried mucilage is affected by the type of mucilage and microorganisms and can vary from isolated local spots, to networks spanning across larger areas of the soil particle surface. However, until now the understanding on how this heterogeneous distribution and its morphology affect infiltration and water repellency in soil is limited.

Therefore, the goal of this study is to investigate the impact of the spatially heterogeneous wettability distributions on the infiltration into soil. For this purpose, we utilize a two-phase flow model based on the Lattice-Boltzmann to numerically simulate the infiltration in porous media with a simplified geometry and for different selected heterogeneous wettability coatings. Additionally, we simulated the rewetting of dry rhizosphere of a sandy soil where dry hydrophobic mucilage depositions on the particle surface are represented via a locally increased contact angle.

Our simulations show that water repellency in porous media can occur not only when the soil particles are hydrophobic but also when their wettability is reduced on small local spots. In particular, we can show that the hydraulic dynamics and effective water repellency are determined by the specific location within the pore space where wettability is reduced or hydrophobic, rather than by the averaged contact angle. This raises questions about the applicability of the Cassie equation that considers only an averaged contact angle to most porous media, since for instance, coatings in the pore throat and pore body often have different effect strengths. Thus, within the rhizosphere, even relatively small areas coated with dry hydrophobic mucilage in the pore throats can cause water repellency in an otherwise well-wettable and water-conducting soil.

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MS10 / 217

## How to capture centimeter-scale local variations in the pore space of paper: A benchmark study using $\mu$ -CT

**Authors:** Matthias Neumann<sup>1</sup> ; Eduardo Machado Charry<sup>2</sup> ; Ekaterina Baikova<sup>2</sup> ; André Hilger<sup>3</sup> ; Ulrich Hirn<sup>4</sup> ; Ingo Manke<sup>3</sup> ; Volker Schmidt<sup>1</sup> ; Karin Zojer<sup>2</sup>

<sup>1</sup> *Institute of Stochastics, Ulm University, Ulm, Germany*

<sup>2</sup> *Christian Doppler Laboratory for mass transport through paper and Institute of Solid State Physics, Graz University of Technology, Graz, Austria*

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Though X-ray microcomputed tomography ( $\mu$ -CT) is an established and versatile tool to determine the 3D microstructure of porous materials, it is still a major challenge to capture the degree of disorder and to determine the extent of heterogeneity in membrane-like materials [1,2]. Membranes, such as paper sheets, possess enormous aspect ratios. The formation of paper sheets yields a complex network of fibers that is characterized by strong local variations across the sheet, as found for fiber-based microstructures in general [3]. For properties associated with the pore space of paper, the impact of local in-plane variations, e.g. due to regions where fiber accumulations occur, is not well established so far. Hence, paper and particularly its pore space is an elegant test bed for designing and performing a  $\mu$ -CT-based microstructure acquisition that is capable of revealing sheet-representative in-plane variations up to the centimeter range and variations in the sheet cross-sections within a few micrometers or less.

A framework to analyze local variations in the microstructure of paper sheets based on 3D image data is presented. To this end, a workflow to efficiently acquire a large set of highly-resolved tomographic image data is developed. In combination with statistical image analysis, this enables the quantification of local variations and pairwise correlations of morphological microstructure characteristics on length scales ranging from micrometers to centimeters. The microstructure characteristics considered in the present study are porosity, thickness, and mean geodesic tortuosity quantifying the length of the shortest transportation paths in the pore space [4]. The power of the presented framework is demonstrated by (i) quantitatively revealing the difference in terms of local structural variations between a model paper before and after unidirectional compression via hard-nip calendering as well as (ii) determining the field of view, which is required to reliably compute the local probability distributions of the considered microstructure characteristics. On the basis of our comprehensive data sets, relationships between structural differences and local densifications are elucidated. In particular, it is shown how calendering transforms local variations in sheet thickness into marked local mass density variations. The obtained results are in line with experimental measurements of macroscopic properties (basis weight, Bekk smoothness parameters, thickness, Gurley retention times) determined for the considered paper materials.

[1] W. M. Harris and W. K. S. Chiu, *J. Power Sources*, 282:622–629, 2015;

[2] R. Banerjee, J. Hinebaugh, H. Liu, R. Yip, N. Ge, and A. Bazylak, *Int. J. Hydrog. Energy*, 41, 14885–14896, 2016.

[3] J. Dirrenberger, S. Forest, and D. Jeulin, *Int. J. Solids Struct.* 51, 359–376, 2014.

[4] M. Neumann, E. Machado Charry, K. Zojer, and V. Schmidt, *Methodol. Comput. Appl.*, 2021, doi:10.1007/s11009-019-09761-1.

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MS1 / 524

## Hydrate formation and migration in stratified porous media

**Authors:** Tianjia Huang<sup>None</sup>; Ke Xu<sup>1</sup>

<sup>1</sup> *Peking University*

**Corresponding Authors:** kexu1989@pku.edu.cn, huangtj@tamu.edu

Methane often generates in fine-grained marine muds by the biodegradation of organic matter but accumulates in neighboring coarse sand layers in the form of hydrates. This phenomenon is attributed to the higher capillary pressure in mud layers than in sand layers, which makes hydrate accumulation in sand layers more thermodynamically favorable. However, rarely explored is its kinetics, i.e., how fast is methane to migrate from where it generates to where it finally accumulates. We investigate the hydrate formation and migration kinetics in stratified porous media, using a novel 1-D diffusion-reaction model. This model counts Non-Fickian diffusion induced by the temperature gradient, gravitational effect, and capillary pressure gradient, which have not been considered simultaneously in previous studies.

We first investigate a simplified scenario that consists of two neighboring mud and sand layers with identical thickness and porosity. In this scenario, capillary pressure contrast dominates over all other non-Fickian diffusion mechanisms, so the model can be highly simplified that allows for analytical solutions. A modified  $Da$  number is defined to characterize the ratio between methanogenesis rate and migration rate, that divides the methane migration kinetics into two regimes: when  $Da < \sim 0.4$ , hydrate never cumulates in the mud layer but directly cumulates in the sand layer; when  $Da > \sim 0.4$ , hydrate first cumulates in the mud layer but gradually migrates to the sand layer. For the latter regime, a critical time  $t_c$  is identified, after which the sand layer cumulates more hydrate than the mud layer. The above analytical results match the full numerical solution well. The analytical prediction of critical  $Da$  and  $t_c$  matches well with the full numerical solution.

We further conduct full simulation on a much larger system that consists of multiple different sedimental layers. The accurate description of this process requires all non-Fickian diffusion mechanisms to be accounted for. The results show that gravitational and thermal gradient gradually dominates over capillary contrast in larger temporal and spatial scales, while capillary pressure still depicts local features of hydrate distribution.

This work systematically illustrates general principles of how the interplay between methane generation and migration controls hydrate saturation profile evolution in stratified porous media, which further helps in the evaluation of hydrate exploitation's feasibility.

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MS21 / 496

## Hydraulically driven fractures in deformable porous media- Impact of non-linear flow patterns in vicinity of fractured zone

**Author:** Nima Sarmadi<sup>1</sup>

**Co-author:** Mohaddeseh Mousavi Nezhad<sup>2</sup>

<sup>1</sup> *University of Warwick*

<sup>2</sup> *Associate Professor*



**Corresponding Authors:** m.mousavi-nezhad@warwick.ac.uk, nima.sarmadi@warwick.ac.uk

Predicting mutual fluid-solid interactions in subsurface reservoirs is essential to address critical geoscientific challenges related to geo-energy such as geothermal energy, hydrocarbon exploration, and underground storage sites. In this work, a mathematical setting is presented on the basis of the variational principle for the minimisation of fracturing system energy in the context of finite strain elasticity. The nonlinear system of equations is solved by employing an iterative Newton method on the finite element mesh to emulate nonlinear hydro-mechanical processes of the subsurface porous materials, and the robustness of this numerical method is tested by simulating a benchmark example. The particular focus is on investigating the impact of the non-linear flow field within the fractured zone, the prediction of the fracture pathway, and the evolution of reservoir transmissivity. The results imply the significant changes of the fluid regime and the pressure drop inside the crack as well as around the crack-tip caused by the development of fracture subjected to fluid injection.

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**Poster + / 603**

## **Hygromechanical Properties of PEG-Treated Archaeological Wood: Molecular Simulation and Poromechanics**

**Author:** Ali Shomali<sup>1</sup>

**Co-authors:** Chi Zhang<sup>2</sup>; Eleanor J. Schofield<sup>3</sup>; Benoit Coasne<sup>4</sup>; Dominique Derome<sup>5</sup>; Jan Carmeliet<sup>6</sup>

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<sup>2</sup> *ETH zurich*

<sup>3</sup> *The Mary Rose Trust*

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Archaeological wood of shipwrecks buried for centuries under sea sediments is highly degraded due to the chemical changes and material loss. Uncontrolled or rapid drying of such artifacts results in drastic distortion and collapse of material due to high drying stress, therefore consolidation methods and drying processes have been developed to preserve these culturally valuable artifacts. As a consolidation technique used for both Swedish warship *Vasa* [1] and Henry VIII's warship the *Mary Rose* [2], polyethylene glycol (PEG) solution was sprayed for decades on the surface of both shipwrecks to penetrate the wood and stabilize the wood structure [1]. While the experimental results show higher stability in PEG-treated samples [1], many questions regarding the impact of PEG polymers on the stability of wood polymers remain unanswered due to the microscopic nature of complex nanoscale phenomena involved. In this study, we combine the data obtained from molecular dynamics (MD) and grand canonical Monte Carlo (GCMC) simulation with a poromechanical model to examine the PEG-cellulose synergic interaction in amorphous mixtures as observed in sorption isotherms, mechanical moduli and hydrogen bonding network. To this aim, mixtures of amorphous cellulose and PEG200 are constructed as simple models representing the interaction of PEG200 consolidant with cell wall holocellulose component. Mixtures with different mass ratios of cellulose and PEG are modeled using the OPLS-AA force field and prepared by high-temperature relaxation followed by quenching at room temperature. Hybrid MD/GCMC is then employed to obtain the sorption isotherms and PEG-cellulose mixtures at different levels and regimes of hydration. Following the

GCMC simulations, mechanical tests are performed on resultant structures to examine the sorption-induced mechanical softening in the wood structure for both treated and untreated samples. The data are then introduced into a poromechanical model which allows analyzing the change in the coupling between sorption and deformation by adding PEG to cellulose. The presented model, methodology, and the choice of simulation parameters such as system size are validated through comparison with available simulation and experimental data on amorphous cellulose sorption isotherms and mechanical properties. As indicated by sorption isotherms and swelling curves, the PEG-cellulose mixture shows deviation from the ideal mixture rule referring to a synergic interaction between PEG and Cellulose. This synergic behavior can be examined by investigating the confinement of PEG molecules in the nanoporous structure of amorphous cellulose and by the hydrogen bonding network between cellulose and PEG. The PEG molecules rearrange the existing hydrogen bonding network by forming new hydrogen bonds with the cellulose chains reducing the sorption sites available for moisture adsorption. In addition, the amorphous cellulose limits the free swelling of PEG observed in its pure liquid form. These two mechanisms can describe the reduction in moisture content and its outcome: less swelling/shrinkage in treated samples and thus higher stability in museum conditions.

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Time Block B (14:00-17:00 CET) **References:**

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## Hygromechanical mechanisms of wood cell wall revealed by molecular modeling and mixture rule analysis: Role of components, interphases and hydrogen bonding

**Authors:** Chi Zhang<sup>1</sup> ; Sinan Keten<sup>2</sup> ; Benoit Coasne<sup>3</sup> ; Dominique Derome<sup>4</sup> ; Jan Carmeliet<sup>5</sup>

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Wood is a natural porous bio-polymeric material with complex hierarchical structure. Owing to its exceptional mechanics and sustainability, wood has been an essential material for mankind, in both conventional applications, e.g. building material, and future advanced systems, e.g. green electronics. Sorption of environmental moisture strongly affect wood mechanics, due to the intrinsic nanoscale porosity and hydrophilicity of wood cell wall material. Despite the numerous studies on wood mechanics, fundamental mechanical aspects of moisture-induced phenomena such as swelling, weakening, shape memory effect, etc, remain to be fully elucidated in view of wood hierarchical structure.

For investigating the wood cell wall nanostructure and the physical nature of wood-water relationship, this study presents a state-of-the-art atomistic model of softwood cell wall layer, taking great care to reflect the state of knowledge of wood molecular structure. Individual polymer components, their mixtures, composites and interfaces are mechanically characterized in separate simulations, gathering an unprecedented micromechanical dataset including hydrogen bonding, swelling and weakening, over the full hydration range. Quantitative agreement with available experimental reports is achieved. Based on the rich dataset, material models based on mixture rule uncover the

impact of intermolecular interactions and identify the role of different components and their interactions with water. The most critical factors determining wood mechanics on the nanometer scale, and in particular the pivotal role of interphases, indicating an interaction between different polymeric components, are highlighted. Especially, it is shown that the hemicellulose glucomannan plays the role of a glue between the reinforcing crystalline cellulose and other matrix components, showing a moisture-sensitive anisotropic interphase zone. The work gives thought to the origin of wood cell wall orthotropy, moisture-induced weakening and swelling, each a different manifestation of the strong coupling between the mechanical and hygric behavior of wood.

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MS11 / 488

## Ice crystallization and mechanical damage at the pore scale

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### Ice crystallization and mechanical damage at the pore scale

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**Abstract**

Frost in wintry weather conditions is one of the major causes of the degradation of roads, buildings and outdoor artworks that are all porous media and are prone to damaging. With the decrease of the temperature, the water present in the porous structure can crystallize; the formation of ice in the pore network or in cracks subsequently results in mechanical damage such as crack propagation or the delamination of the stone. The effect of ice crystallization in unconsolidated porous materials, known as frost heaving, results in an upward swelling of soils during freezing. Previous studies on freeze/thaw cycling in porous media have been done mostly on the macro and mesoscale. However, the detailed mechanism by which the damaging occurs is still ill understood; for instance, the mechanical properties of the ice and most porous media are such that one would expect the ice to break, and not the porous medium to be damaged.

Here, we present our results on ice crystallization in confinement at the microscale and investigate the conditions under which mechanical damage develop. In order to do so, micro scale experiments have been performed in a model microcrack/pore. Using glass micro capillaries of various sizes, parameters that cause fracture in the glass capillaries during freeze /thaw cycles are investigated; we are able to freeze water droplets inside the micro capillaries and simultaneously image the freezing and measure the deformation of the capillaries upon freezing, over multiple cycles. From the deformation of the capillaries we can estimate the pressure build-up by the ice in the confinement. The experimental results are compared with theoretical arguments in order to better understand the frost action at microscale on the resulting macroscale mechanical damage. The hoop stress responsible of the breaking of a single pore has been calculated considering the pressures induced by the crystallization process and the volume expansion of liquid water turning into ice.

Finally, we will discuss the importance of contact angle, volume of the confined water as well as the cycling on fracture observed in microcapillaries.

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## Identification of transport and clogging parameters of porous media

**Authors:** Boris Maryshev<sup>1</sup> ; Anna Evgrafova<sup>1</sup> ; Nikolay Kolchanov<sup>1</sup> ; Mikhail Khabin<sup>1</sup>

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Most natural porous media have a rather complex structure. Usually the solute transport in a porous medium is described within the framework of the standard diffusion model [1]. However, many experimental data [2, 3] cannot be explained into frameworks of such approach, because the transport through a porous medium is often complicated by the immobilization of solute. The immobilization leads to a change in the effective pore size, and it means the variation in the permeability of the medium. The change in permeability, in turn, leads to a change in the filtration rate. There are several of the most popular models describing the processes of solute immobilization during filtration through a porous medium [4-6].

In this work, the process of solute transport through a porous medium is experimentally studied. The experimental setup is constructed from a copper tube filled with a porous medium. Glass balls are used as porous filler. This is the most affordable filler option with well-controlled grain size. Distilled water is pumped through the tube, pumping is carried out with a constant pressure drop between the inlet and outlet. The pumping of a clean liquid is carried out until complete saturation of the medium. The saturation control is performed by the electronic balance, with an accuracy of at least 1%. A pumping of constant concentration NaCl solution starts in initial time moment. Simultaneously, the measurement of NaCl concentration and mixture flow rate at the outlet begins. The measurement is carried out continuously until the registration zero concentration and constant flow rate. As the result the breakthrough curve and the dependence of flow rate in time is obtained for each value of pressure drop and NaCl concentration.

To estimate the transport parameters of the medium, a one-dimensional problem of the solute transport was solved numerically. Darcy's equation [7] was used to model the flow in a porous medium. It was assumed that the permeability is an unambiguous function of the porosity of the medium (the measured porosity of the pure medium is 0.37). To model this dependence, the Kozeny-Karman relation was used [8]. The solute transport was modeled within the MIM approach with taking into account the saturation of immobile phase and linear kinetics of desorption [5]. It was assumed that in this case the porosity of the medium decreases in proportion to the volume concentration of the adsorbed solute. Thus, when solving the described problem, it is possible to obtain the dependence of the solute concentration and the flow rate at the outlet on time. Based on the comparison of the experimental data with the data obtained in the course of numerical simulation, we solve inverse problem of identifying the transport parameters of the medium. The values the sorption coefficients, the effective diffusion coefficient were obtained. It is also shown that within the limits of the method error, these parameters are practically independent of the pressure drop and the solute concentration at the inlet.

The work was supported by the Russian Science Foundation (Grant No. 20-11-20125)

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## Image Segmentation with Transfer Learning for Carbonate Rock Images

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**Abstract—** The approach of using machine learning related or deep neural networks for semantic segmentation has highly been successful in various areas of research irrespective of the levels of complexity of the structural patterns involved in images of interest. With the adoption of unsupervised learning, human-related errors in segmentation may be suppressed and process time saved. However, it should be noted that machine or deep learning related approaches demand large datasets for training and high computational resources due to the huge numbers of training parameters and image samples.

In this study, we explore the implementation of transfer learning, using pre-trained networks VGG16 [1] and MobileNet-V2, into end-to-end semantic segmentation architectures proposed in the literature, i.e. SegNet [2] and UNet [3], respectively. We implement this study on highly heterogeneous real rock 2D carbonate images from our laboratory, to evaluate a number of evaluation metrics including precision and recall, and compare to verify the effectiveness of the binary cross-entropy and dice loss functions on image semantic segmentation. We also evaluate and compare the porosity prediction results using segmented images from the proposed models as a measure of evaluating the influence of transfer learning on deep learning-based image segmentation.

Results show that the state-of-art transfer learning, responsible for the transfer of learned weights into a new training environment is able to reduce model training computation time and the number of rock image samples required for training. We are also able to achieve the intended training performance, relatively comparable to that obtained from the originally proposed networks, i.e., SegNet [2] and UNet [3] with a limited number of training samples. Our results show comparable rock porosity predictions between the ground truth, original and proposed model predictions.

**Time Block Preference:**

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## Image-based modeling of spontaneous imbibition in porous media

**Authors:** Chao-Zhong Qin<sup>1</sup>; Xin Wang<sup>1</sup>

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The dynamic pore-network modeling [1-3], as an efficient pore-scale tool, has been used to understand imbibition in porous media, which plays an important role in many subsurface applications. In this talk, we will present a dynamic pore-network model for imaged-based modeling of spontaneous imbibition in porous media. The  $\mu$ CT scanning of a porous medium of sintered glass beads is selected as our study domain. We extract its pore network by using an open-source software of PoreSpy, and further project the extracted information of individual watersheds into multiform idealized pore elements. A number of case studies of primary spontaneous imbibition have been conducted by using both the pore-network model and a VOF model, under different wettability values and viscosity ratios. We compare those model predictions in terms of imbibition rates and temporal saturation profiles along the flow direction. We show that our pore-network model can well predict imbibition rates and temporal saturation profiles under different viscosity ratios and wetting conditions, in comparison to the VOF model. We explore the effect of viscosity ratio on the entrapment of nonwetting phase. Moreover, we discuss the difference between spontaneous imbibition and quasi-static imbibition in terms of pore-filling mechanisms.

### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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## Image-based morphological characterization of multiphase porous media flow

**Authors:** Samaneh Vahid Dastjerdi<sup>None</sup>; Nikolaos Karadimitriou<sup>1</sup>; Holger Steeb<sup>2</sup>

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Understanding the physics of immiscible two-phase flow in porous media is not a straightforward process due to the large number of influencing factors. Such factors are, among others, the inherent fluid properties, the solid-fluid interactions, the properties of the solid structure, and the boundary as well as the initial conditions. Since two-phase flow has a significant impact on many applications, such as geological carbon sequestration (GCS), enhanced oil recovery (EOR), and non-aqueous phase liquid (NAPL) contamination of groundwater and consequent soil remediation, it is of great interest to elaborate further on these aspects and to understand the underlying pore-scale physics.

Given the pronounced effects of the pore-scale geometry and the pore-fluid configuration on two-phase flow, various attempts have been made to embed these parameters on the continuum scale, i.e., mean-field, models. However, even in the best-case scenario, these models fail to incorporate the effect of small-scale topological features of the fluid phases, e.g. phenomena related to trapping mechanisms (like wetting cones, single ganglia or films, which are typical for disconnected phases) in the evolution of flow.

One of the existing approaches used in the prediction of the configuration of fluids in a porous medium, was proposed by Lenormand et al. [1]. The Lenormand phase diagram relates the capillary number ( $Ca = \mu_n q / \sigma_w n$ ) and the mobility (or: viscosity) ratio ( $M = \mu_n / \mu_w$ ) with the three characteristic displacement regimes in a porous medium. However, this approach does not account for the structure of the flow domain at all.

In order to put Lenormand's phase diagram to test with regards to the pore structure and identify the effect of the geometrical characteristics (e.g. the pore and throat size distribution, or the porosity and connectivity) of each domain on the evolution of flow, two-phase flow experiments are performed for various pore structures as well as several capillary number/viscosity ratio combinations. Micromodels, employed in the experiments are either made of PDMS (Poly-Di-Methyl-Siloxane) [2] or glass (commercially available). The transparency of the micromodels facilitates the experiments with real-time pore scale visualization of two-phase displacement and the processes involved.

An image-processing tool has been developed and applied, in order to segment and analyze the microscopic images which are acquired. From the segmented images, the local and REV-scale capillary pressure is calculated and the Euler characteristics (obtained from the Minkowski functionals, i.e.,  $M_0 \sim M_3$  [3],[4]) as a measure of topological assessment of the flow process is determined. Furthermore, the discontinuities occurring during the flow process can be classified into cones, films and pendular disconnections and used as another characterization criterion.

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## **Imbibition Effect and Driving Mechanism of Nanofluid in Porous media**

**Authors:** Rundong Qiu<sup>None</sup> ; C.Y. Gu<sup>None</sup>

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The imbibition mechanism is the basis for efficient development of unconventional dense reservoirs and it is the key to clarify the imbibition mechanism to find out the driving forces of oil imbibition in porous media. Based on MRI and static permeation test, the In-situ changing images of oil in different cores from ultralow permeability to high permeability were obtained for 200h days. These in-situ diagrams can well explain the driving force of the imbibition of crude oil in different permeability cores.

The test results show that the oil distribution map of high and medium permeability core is stronger from bottom to top, the oil drainage of low permeability and ultra low permeability core is slow, the oil recovery is low, and there is no obvious difference between upper and lower oil distribution images, but gradually fade from peripheral to inner.

Theoretical studies show that oil droplets are mainly affected by differentiation force (i.e. buoyancy and gravity difference), capillary force (i.e. deformation capillary resistance and pore wall viscous capillary resistance), while the main driving force of oil drainage in different permeability cores of nanofluids is different. The capillary resistance in high and medium permeable rock is small, the differentiation force is the dominant driving force, and the oil droplet is subjected to upward movement from bottom to top. The capillary resistance of the porous core is large, and the differentiation force is difficult to push the oil the oil droplet out. The imbibition mainly depends on the spontaneous equilibrium of the three-phase interface and internal diffusion to produce droplet exchange, which gradually weakens from inside to outside.

Therefore, the theoretical analysis is consistent with the NMR. Nanofluids can enhance core hydrophilicity and reduce oil-water interfacial tension, and accelerate the spontaneous balance of three-phase interface and reduce capillary force, which is beneficial to stripping oil droplets from core wall. Therefore, nanofluids can improve the efficiency of oil drainage, whether for high permeability cores or ultra-low permeability cores.

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## Imbibition-Induced Deformation in Nanoporous Vycor Glass

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We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (Vycor glass) upon spontaneous, capillarity-driven infiltration of water. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformation originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime) upon water invasion, whereas the second results from Laplace pressure effects [1,2,3]. Our study demonstrates that it is possible to monitor imbibition dynamics by simply dilatometry measurements.

**Time Block Preference:**

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# Impact of Multi-scale Deformations on Multiphase Flow Considerations in Porous Media

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Subsurface processes reflected in groundwater hydrology in the vadose zone, geological CO<sub>2</sub> sequestration, transport of non-aqueous phase liquid contaminant in aquifers, extraction of geothermal energy and enhanced oil recovery require an accurate characterization of mechanical pore deformation, multiphase fluid transport, and their physical interactions (i.e., poromechanical interactions). Recognizing that the subsurface will also be exploited as an energy storage resource as society makes a transition to renewable energy sources, an improved understanding of the imposed coupled hydraulic, thermal, mechanical and chemical processes is required to ensure the subsurface is developed in a safe, secure manner. Pore-spaces present within these subsurface formations will deform in response to the changes in effective stress, and in general, the physical mechanisms controlling stress-dependent pore deformations are well-understood, both analytically (based on poroelasticity theory), and experimentally. These poromechanical interactions have been shown to have a major impact on single-phase (i.e., absolute permeability) and multiphase flow properties of porous media and so it is expected that multiphase flow mechanisms including drainage and imbibition would also be expected to be deformation-dependent in porous media. Today, sophisticated models are being developed and implemented that can capture complex multiscale, multiphysics phenomena but rarely do these models incorporate dynamic changes (i.e. pore volume and topology changes due to changes in effective stress) in relative permeability and/or capillary pressure relationships. This presentation will explore recent experimental studies that have revealed significant impacts on the multiphase flow properties (e.g., relative permeability and capillary pressure) of rocks as a result of effective stress-induced pore deformation and the impacts on modeling from the pore network scale to reservoir scale will be discussed in relation to these studies.

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MS8 / 301

# Impact of Physical Heterogeneity on Effective Reaction Rates

**Authors:** Rodolfo Oliveira<sup>1</sup> ; Martin Blunt<sup>1</sup> ; Branko Bijeljic<sup>2</sup>

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Reactive transport in porous media is of key importance in contaminant hydrology, carbon storage, enhanced oil recovery and chemical reactors engineering. Despite progress made in recent decades, measurement and prediction of the effective reaction rates is still not well understood. In this study we show how flow and transport heterogeneity affects the effective reaction rate. Our approach is based on a reactive transport particle tracking model at the continuum scale, in contrast to the pore-scale models which were successfully used to study the impact of heterogeneity on non-Fickian transport (Bijeljic et al., 2011, 2013) and reactive transport (Pereira Nunes et al., 2016). We make use of our reactive continuous time random walk (CTRW) model that was previously validated using Nuclear Magnetic Resonance (NMR) experimental measurements during dissolution of a Ketton carbonate rock core sample (Oliveira et al., 2021). The CTRW model is defined using a truncated power-law distribution of transit-time, which contains diffusive time cut-off, mean advective time, and a parameter  $\beta$  characterising the domains unresolved physical heterogeneities. To systematically study the effects of flow and transport heterogeneities on the effective reaction rates, we construct three domains with increasing physical and transport heterogeneity, and subject each domain to three different advective regimes with  $Pe = 20, 200$  and  $2000$ . This strategy allowed us to examine nine initial states. For transport, we characterize signatures of physical heterogeneity in the three porous media using velocity distributions and show how these imprints on the signatures of particle displacement, namely particle propagators distributions. In addition, we demonstrate the ability of our CTRW model to capture the impact of physical heterogeneity on the longitudinal dispersion coefficient over several orders of magnitude for a wide range of  $Pe$  defining transport regimes. Reactive transport simulations indicate that the effective reaction rates depend on (i) initial physical heterogeneity and (ii) transport conditions. We show that the higher the initial heterogeneity, the lower the reaction rate. Finally, a decrease in  $Pe$  would promote mixing by diffusion over advection, resulting in the higher reaction rates. Overall, we establish a framework to demonstrate and quantify the impact of physical heterogeneity on transport and effective reaction rates in porous media.

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Time Block C (18:00-21:00 CET) **References:**

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MS3 / 112

## Impact of Roughness on Multiphase Fracture Flow - Insights from 3D-Printed Fractures

**Authors:** Tomos Phillips<sup>1</sup> ; Jeroen Van Stappen<sup>2</sup> ; Tom Bultreys<sup>2</sup> ; Stefanie Van Offenwert<sup>2</sup> ; Arjen Mascini<sup>3</sup> ; Shan Wang<sup>2</sup> ; Veerle Cnudde<sup>2</sup> ; Andreas Busch<sup>1</sup>

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**Corresponding Authors:** a.busch@hw.ac.uk, tom.bultreys@ugent.be, shan.wang@ugent.be, tp45@hw.ac.uk, veerle.cnudde@ugent.be, jeroen.vanstappen@ugent.be, arjen.mascini@ugent.be, stefanie.vanoffenwert@ugent.be

Fractures can provide principal fluid flow pathways in the Earth's crust, making them a critical feature influencing subsurface geoenergy applications, such as the storage of anthropogenic waste, emissions or energy. In such scenarios, fluid-conductive fault and fracture networks are synonymous with two-phase flow, due to the injection of an additional fluid (e.g. CO<sub>2</sub>) into an already saturated (e.g. brine) system. Predicting and modelling the resulting (partly-)immiscible fluid-fluid interactions, and the nature of fluid flow, on the field-scale, requires an understanding of the constitutive relationships (e.g. relative permeability and capillary pressure) governing fluid flow on the single-fracture scale. In addition to capillary and viscous forces, fracture relative permeability is influenced by aperture heterogeneity, arising from surface roughness. The degree to which surface roughness controls relative permeability behaviour in fractures remains unclear. As all fractures display roughness to various degrees, furthering our understanding of two-phase flow in fractures benefits from a systematic investigation into the impact of roughness on flow properties. To this end, we performed co-injection experiments on two 3D-printed (polymeric resin) fractures with different controlled and quantified surface roughness distributions (Joint Roughness Coefficients of 5 & 7). Brine and decane were simultaneously injected at a series of incrementally decreasing brine fractional flow rates (1, 0.75, 0.5, 0.25, and 0), at low total volumetric flow rates (0.015 mL/min). Steady-state fluid occupancy patterns, preferential flow pathways and overall fluid saturations in each fracture were imaged and compared using an environmental laboratory-based  $\mu$ -CT scanner with a 5.8  $\mu$ m voxel size (EMCT; Ghent University Centre for X-ray Computed Tomography). Experimental results highlight the importance of roughness on the relative permeability behaviour of fractures, which is, for example, a principal control on leakage rates from geological stores.

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**Poster + / 717**

## Impact of Wettability on Reservoir Quality Distribution and Preservation

**Authors:** stephen Gundu<sup>None</sup> ; Cees Der Land<sup>None</sup> ; Sanem Acikalin<sup>None</sup> ; Tannnaz Pak<sup>None</sup>

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## Impact of operational factors on Aquifer Storage and Recovery (ASR) scheme in saline regions

**Authors:** Shubhaam Tiwari<sup>1</sup> ; Brijesh Kumar Yadav<sup>1</sup>

<sup>1</sup> *IIT Roorkee*

**Corresponding Authors:** brijesh.yadav@hy.iitr.ac.in, stiwari@hy.iitr.ac.in

Groundwater depletion has been significant in the last half century. Different technical developments for expected groundwater replenishment known as managed aquifer recharge have been established to increase the groundwater level. Groundwater salinity is a major problem in many arid and semiarid regions of India where fresh water supplies are limited due to inadequate rainfall and long dry seasons. Modern ASR techniques, in which excess surface water is diverted to the underlying aquifers for eventual recovery, are used to effectively use water supplies in water-scarce areas, including salt-affected zones. The purpose of this study is to gain a better understanding including its operational process of groundwater storage and recovery. The impacts of various operational factors such as injection volume, injection and recovery rates, and storage duration of freshwater within saline aquifer are analysed and results are presented. The findings of this study would have a significant effect on the ASR scheme's operational phase, ensuring its performance and effective freshwater recovery.

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**Poster + / 158**

## Impact of osmosis and emulsification on oil remobilization in pore-scale experiments

**Author:** Lifei Yan<sup>1</sup>

**Co-authors:** Mohammad Hossein Golestan<sup>2</sup> ; Wenyu Zhou<sup>3</sup>

<sup>1</sup> *Utrecht University*

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**Corresponding Authors:** mohammad.h.golestan@ntnu.no, l.yan@uu.nl, wenyuz@stud.ntnu.no

Numerous experimental observations and field applications have confirmed that low-salinity water flooding is an effective technique for enhanced oil recovery. Given the complex physical and chemical processes, several controlling mechanisms have been proposed to explain the oil remobilization due to low-salinity effects. Osmosis and water-in-oil emulsification are among these mechanisms. However, our knowledge of these processes is limited and their associated time scales are not well understood.

To verify their roles, we conducted a series of microfluidic experiments by sequentially injecting high-salinity water, pure or surfactant-added synthetic oil, low-salinity water into the hydrophobized glass-based microchips. Several selected specific areas were continuously observed for over 48 hours, with systems of trapped high-salinity water along the solid grains, low-salinity water in bulk, and sandwiched oil. The systems mimicked the contact status of these three fluids in the natural reservoir. In the experiments using pure oil, we found that the trapped high-salinity water gradually squeezed the sandwiched oil phases out of the pores due to the osmosis induced expansion. The

volume of high-salinity water increased by 22.73% with an average rate of 141.88  $\mu\text{m}^2/\text{hr}$ , which was difficult to rely solely on the diffusion of water in the oil. Therefore, we proposed a hypothesis and developed a coupled water transport model to explain the high-salinity water expansion with a water flux in the oil phase. In the experiments with adding surfactant (SPAN 80) in oil, we observed that the expansion rate of high-salinity water was 2.72 times higher than it without surfactant, meaning that the emulsification contributed to accelerating water transport in the oil phase.

On the other hand, a corresponding series of experiments were carried out using Zetasizer to capture the size trend in water-in-oil emulsion around the oil/salinity-water interface under different salinity conditions. In the case of 1,700 ppm salinity, we found that the water-SPAN80-dodecane emulsions kept a primary size of around 50 nm for the first 4 hours, then generated a second primary size of 2 nm during 4-20 hrs. Finally, the small emulsions progressively dominated the size distribution around the interface, and relative big emulsions, e.g., 4,800 nm, occurred with the coalescence until the emulsification process reached equilibrium. This tendency matched well with the observation on the emulsion transformation in the microfluidic experiments and helped explain the process of high-salinity water expansion.

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Poster + / 269

## Impact of pore-space variations and orientation of layering on the flow properties of Coquina limestone

**Authors:** Mohammad Madankan<sup>1</sup> ; Mehrdad Vasheghani Farahani<sup>1</sup> ; Elli Maria Charalampidou<sup>1</sup> ; Helen Lewis<sup>1</sup> ; Alessandro Tengattini<sup>2</sup> ; Erika Tudisco<sup>3</sup>

<sup>1</sup> *Institute of Petroleum Engineering, EGIS, Heriot-Watt University, Edinburgh, Scotland, UK*

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<sup>3</sup> *Division of Solid Mechanics, Lund University, Sweden*

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In carbonate reservoir rocks, the pore system can vary significantly with variations in the rock component texture and distribution as viewed at different length scales. Any textural variability is reflected in the associated permeability tensor and makes the evaluation of the hydraulic behaviour of this group of rocks very challenging. In this study, we investigated the impact of the core-scale layering orientation to imposed fluid movement direction together with the pore space variations resulting from textural characteristics (inside and outside the layers) on the petrophysical properties and flow behaviour of Coquina limestone. For this analysis, we combine a) X-Ray Tomography (XRT) images (40  $\mu\text{m}$  voxel size resolution) from dry cores; b) Computational Fluid Dynamic simulations; and c) High-Speed Neutron Tomography (HSNT) images (200  $\mu\text{m}$  voxel size resolution) from the same cores during fluid flow experiments. In particular, the 3D pore network extracted from the XRT images was used to characterise the spatial variation of its properties (e.g., porosity, specific surface area, tortuosity and connectivity). Then, the absolute permeability in a number of sub-volumes distributed along the full length of the sample was computed using the Lattice Boltzmann Method (LBM). In this way, the variations in absolute permeability along the sample's length were explored and correlated with pore network characteristics that were previously defined from the XRT. Finally, HSNT images, acquired during flow experiments (injection of heavy water into Decane saturated samples), were further processed to visualise in 3D and time flow patterns within samples containing layering oriented either parallel or perpendicular to the intended injection directions. Results from the pore network characterisation and the LBM simulation revealed significant variations in the pore network properties as well as the calculated absolute permeability of the layers and their

surrounding regions. Those variations were attributed to the orientation of the layers and the textural characteristics of the rock within the tested samples. Two distinct flow patterns were recognized in coquina samples with similar porosity and permeability but with different layering orientation. When layering is oriented parallel to the sample's length (and in the injection direction), the dominant water flow is through the high permeability zones, which are separated from each other by lower permeability layers. This results in unstable advancement of fluid front, shorter breakthrough time and lower differential fluid pressures. On the other hand, when the layers are oriented normal to the intended flow direction the existence of cross-flow layers of reduced porosity and absolute permeability is found to stabilize the flow pattern (piston like) and cause higher differential fluid pressure.

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**Poster + / 351**

## Impact of salt on sorption isotherms in nanoporous media

**Authors:** Hugo Bellezza<sup>1</sup> ; Marine Poizat<sup>1</sup> ; Olivier Vincent<sup>2</sup>

<sup>1</sup> CNRS & Univ. Lyon 1, ILM

<sup>2</sup> CNRS

**Corresponding Authors:** olivier.vincent@univ-lyon1.fr, marine.poizat@ens-paris-saclay.fr, hugo.bellezza@univ-lyon1.fr

Salt water is ubiquitous in nature (e.g. geomaterials, soil, clouds formation) and in technology (e.g. desalination, concrete weathering, heritage conservation). In most of these situations, salt water is confined within a porous medium, often with pores down to the nanometer scale: for example, crystallization and dissolution cycles induced by humidity changes are known to induce structural damage to building materials, artwork, etc. And yet, these processes are not well characterized, especially when pores are in the nanometer range. Here, we investigate the response of the salt water confined in several porous silicon samples (average pore diameter from 3 nm to 20 nm) to humidity cycles. We performed sorption isotherms where we monitored optically water content in the porous medium. We systematically characterized how the salt concentration impacts the shape of the isotherms and compared these results to a minimal model coupling solution thermodynamics to capillarity, nucleation and confinement effects.

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## Implementation of Higher-Order methods for Modeling of the Single-Phase Multicomponent Flow in Porous Media

**Authors:** Petr Gális<sup>1</sup> ; Jiří Mikyška<sup>None</sup>

<sup>1</sup> Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague

**Corresponding Authors:** galispet@fifi.cvut.cz, jiri.mikyska@fifi.cvut.cz

In this work we derive a higher-order numerical scheme for the single-phase multicomponent flow in porous media. The mathematical model consists of Darcy velocity, transport equations for components of a mixture, pressure equation and supplemental constitutive relations. The combination of higher-order discontinuous Galerkin method for the discretization of transport equations and higher-order mixed-hybrid finite element method for the discretization of Darcy velocity and pressure equation is used to obtain the discrete problem. The resulting non-linear system is solved with a new fully mass-conservative iterative IMPEC method. To validate the code and to confirm the expected order of convergence some numerical experiments of 2D flow have been carried out.

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## Implications of plant exudates on the formation of rhizosheaths

**Author:** Riffat Rahim<sup>1</sup>

**Co-authors:** Eva Kroener<sup>1</sup> ; Adrian Haupenthal<sup>1</sup>

<sup>1</sup> Forschungszentrum Juelich

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Root exudates stimulate microbial activity and functions as binding and adhesive agent that increases aggregate stability in the rhizosphere. The exudates produced from plant roots and microorganisms in rhizosphere plays a significant role in the formation of rhizosheath. A high viscosity stabilizes soil aggregates in the surrounding of the root and creates rhizosheath. The formation and stabilization of rhizosheath of maize plants under various soil water contents has been studied in the past but the influence of root exudates on the rhizosheath formation associated with other rheological properties still needs to be investigated and understood. Such knowledge will greatly enhance the understanding of how rhizosheath is formed under different root and seed exudates and effect of their physio-chemical properties on the adhesion properties of mucilage. The aim of this study is to provide the first combined quantitative data on how root and seed exudates of different plants affects rhizosheath formation. We hypothesized that mucilage will contribute in the formation of rhizosheaths. For this we used the mucilage of chia seeds which acts as a modelled plant root mucilage and mix it with soil in a five different concentration. After preparing the soil with mucilage, artificial roots (flax cords) are incorporated in this soil. After 48 hours at 25°C roots are removed and rhizosheath is measured. For further studies, rhizosheath after drying and wetting cycles, mucilage adhesion, simulation and rheological properties will be investigated under various soil water contents, soil texture, soil type and soil compaction.

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MS10 / 86

**Improved Watershed-based Pore Space Partitioning Algorithm for Pore Network Modelling****Authors:** Zeyun Jiang<sup>None</sup> ; Rink van Dijke<sup>None</sup>**Corresponding Authors:** r.van\_dijke@hw.ac.uk, zeyun.jiang@hw.ac.uk

In recent years, watershed-based methods mimicking basin flooding have been adopted for the partitioning the pore space in 2D and 3D images into pores regions as a basis for pore network modelling. However, due to the noisy nature of tomographic images and the neglect of both the convergent and divergent features in different locations in the pore space, watershed-based partitioning algorithms often result in an excessively large numbers of pores, referred to as over-segmentation. Many of these pore regions are redundant with respect to the topology of the pore space and do not notably improve the geometrical characterisation required for, in particular, multi-phase flow simulations. Although some recent algorithms employ additional, usually post-processing, rules to reduce the over-segmentation these still preserve too many unnecessary pores, thus significantly prolonging fluid flow simulations. In this work, we propose a new algorithm to minimise the number of so-called seeds from which the regions grow. Using an efficient region-growing procedure, the algorithm then determines the locally narrowest pore space constrictions separating the pore regions, which in turn map onto the network bonds and nodes, respectively. We combine this new algorithm with an existing medial-axis-based pore network extraction technique (Jiang et al., 2007) facilitating accurate determination of node and bond flow properties, such as capillary entry pressures and conductances. The proposed partitioning algorithm is convincingly validated in terms of pore-by-pore fluid occupancy, as determined by capillary entry pressures, against phase distributions of two-phase flow experiments, visualised directly in a micromodel and in a carbonate rock through synchrotron X-ray micro-tomographic imaging. This demonstrates that the algorithm facilitates highly accurate and highly efficient pore-network simulations.

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MS9 / 404

**Improved micro-continuum formulations for pore-scale simulation of mineral dissolution****Authors:** Cyprien Soullaine<sup>1</sup> ; Julien Maes<sup>2</sup><sup>1</sup> CNRS - Universite d'Orleans<sup>2</sup> Heriot-Watt University**Corresponding Authors:** cyprien.soullaine@cnrs-orleans.fr, j.maes@hw.ac.uk

Mineral dissolution is relevant to most subsurface processes, including CO<sub>2</sub> storage, geothermal systems and enhanced oil recovery. Pore-scale simulation can be a useful tools to decipher the reactive transport within the pore-space and estimate upscaled parameters such as permeability and reaction constants. These simulations may be challenging though as they involve the tracking of multiple solid interfaces. The micro-continuum method is an efficient approach as it does not involve complex algorithms for explicit reconstruction of the interface, but use volume-averaging of the fluid and



solid properties. However, there are two fundamental issues with the current formulation: the need of an interface localisation function to avoid local negative porosity, and concentration bleeding into the solid phase. These two issues lead to significant underprediction of the reaction rate, especially in the diffusion-limited regime, and the reaction constant usually needs to be fitted. To solve these issues, we propose new formulations using a mass conservative localisation function based on the divergence and using the Continuous Species Transfer (CST) method to insure a zero concentration in the solid phase. Our improved formulations are validated by comparison with experimental results and with numerical simulations using a direct method and using the standard micro-continuum approach. We then performed numerical simulations in porous media images and we show that our novel method is as accurate as direct methods and orders of magnitude faster.

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Poster + / 674

## Improvements of stochastic simplex approximate gradient (StoSAG) for production optimization

**Authors:** Xu Jianchun<sup>None</sup> ; Zhou Wenxin<sup>None</sup>

**Corresponding Authors:** 1193398441@qq.com, 472661375@qq.com

StoSAG is an important method to solve optimization problems in reservoir management. But it also faces a major problem-falling down in local optima. We propose some improvements of StoSAG. First, we study the effect of the ensemble number, the cut step number, the initial ensemble, and the initial step size on final optimization value. The performance of the StoSAG is tested on 48 common benchmark functions and compared with the performance of particle swarm optimization (PSO) algorithm. Second, the rules to choose the optimal ensemble number, cut step number, initial ensemble, and initial step size are given considering different function characteristics. The improved StoSAG achieve the best results on all test functions. Finally, the improved algorithm is applied to the optimization of water flooding reservoir model including 10 injectors and 10 produces. By using the improved StoSAG, the NPV is converged to a highest value than both StoSAG and PSO.

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MS14 / 693

## Improving the accuracy of multiscale methods with informed interface spaces based on physics

**Author:** Fabricio Sousa<sup>1</sup>

**Co-authors:** Franciane Rocha<sup>1</sup> ; Roberto Ausas<sup>1</sup> ; Gustavo Buscaglia<sup>1</sup> ; Felipe Pereira<sup>2</sup>

<sup>1</sup> *University of Sao Paulo*

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Simulations of petroleum reservoirs deal with highly heterogeneous permeability fields with multiple scales and high contrast. Multiscale methods are frequently used to simulate such reservoirs because of the huge meshes involved. We discuss here multiscale methods based on domain decomposition, for which the accuracy strongly depends on the interface spaces, i.e., the discrete spaces chosen to represent the variables on the skeleton of the decomposition. We introduce interface spaces based on the geometry of the heterogeneities, especially designed to deal with permeability fields containing high-contrast channelized features such as fractures (high-permeable) and barriers (low-permeable). A pressure space is designed so as to accommodate fractures and a flux space to accommodate barriers. We combine these new interface spaces with the Multiscale Robin Coupled Method (MRCM, [1]), which allows for the independent choice of the pressure and flux interface spaces. The adaptivity of the MRCM is used to automatically select the appropriate parameters at each location, considering the simultaneous presence of fractures and barriers. Our numerical simulations of single-phase and two-phase flows have shown that the MRCM combined with the proposed interface spaces yields promising results for challenging high-contrast porous media problems.

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[1] R.T. Guiraldello, R.F. Ausas, F.S. Sousa, F. Pereira, and G.C. Buscaglia. The multiscale Robin coupled method for flows in porous media. *J. Comput. Phys.*, 355:1-21, 2018. **Acceptance of Terms and Conditions:**

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**Poster + / 694**

## Improving the reliability of phase segmentation by combining 3D imaging and machine learning methods

**Authors:** Parisa Asadi<sup>None</sup> ; Lauren Beckingham<sup>None</sup>

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X-ray CT imaging, which provides a 3D view of a sample, is a powerful tool for investigating the internal features of a porous rock. Classifying phases in these images is highly desirable but, like any other digital rock imaging technique, is time-consuming, labor-intensive, and subjective. Combining 3D X-ray CT imaging with machine learning is a promising, powerful method that addresses the key challenges. This method also makes it possible to simultaneously consider several extracted features in addition to the original images for a more reliable phase segmentation. This study investigates the performance of several filtering techniques with three machine learning methods and one deep learning method to assess the potential for reliable feature extraction and pixel-level phase segmentation of a Marcellus and a Mancos shale. The extracted features are produced by applying image filtering techniques, such as Gaussian and Median, to X-ray CT images and evaluated to determine the best ones to use as feature inputs for machine learning algorithms to obtain more accurate phase segmentation. Three machine learning methods including k-means clustering (k-means), Random Forest (RF), and Feed forward Artificial Neuron Networks (FNN), as well as the deep learning U-Net model, are applied to the original images and the stacked extracted features and their performance compared and contrasted. The results show that all classification algorithms deliver high accuracy ranging from 0.87 to 0.96 when considering more dimensionality (i.e., more features). RF demonstrates the best performance among the machine learning models, with an accuracy of 0.96, due to its capability to handle imbalanced datasets and data scarcity. The U-Net model outperforms the RF model when applied to the test images. ML-based phase segmentation of X-ray CT images enables

faster data collection and interpretation than traditional methods. Considering more dimensionality (i.e., more features) provides promising and reliable segmentation results that are valuable for analyzing the composition of dense samples, such as shales, which are significant unconventional reservoirs in oil recovery.

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MS1 / 673

## In situ study of 3D fluid fingering in porous media using X-ray Computed Tomography

**Author:** Athanasios Papazoglou<sup>1</sup>

**Co-authors:** Barbara Fayard<sup>1</sup>; Jean Doucet<sup>1</sup>; Olivier Guiraud<sup>1</sup>

<sup>1</sup> *Novitom*

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Carbon capture and storage (CCS) is recognized as one of the most effective technologies for reducing CO<sub>2</sub> emissions in the short to medium term. This three-phase process that includes: (i) capture of CO<sub>2</sub>, (ii) transportation, and (iii) underground injection of CO<sub>2</sub> into the geological formations for storage, has highlighted that subsurface energy technologies will play a central role in the transition towards a lower-carbon future. Carbon dioxide geo-sequestration into underground reservoirs is a promising solution to mitigate irregularities in energy production and consumption cycles. Thus, the knowledge of the CO<sub>2</sub>-induced interactions for CO<sub>2</sub>-brine-rock systems at elevated temperatures and pressures, as well as the hydro-mechanical properties of the reservoir, is a requirement for any secure operation of a storage site.

The interactions between the invading and the resident fluid can, under favorable conditions, induce local instabilities in the fluid migration patterns. In particular, inside a porous medium, multi-phase flow is controlled by several factors, including the characteristics of the porous medium and the fluid properties. Studies for such a complex three-dimensional phenomenon have predominantly been performed in two-dimensional laboratory settings. However, to understand and possibly control the micro-scale migration of fluid fingering in porous media, a set of 4D experiments is necessary.

In this context, a series of experiments are performed, focusing on the migration of two immiscible fluids, characterizing percolation modes, and fingering effects developing at different flow conditions. During this process, x-ray tomographies are acquired. The 3D tomographic reconstructed images provide unprecedented insight into the nature and complexity of hydro-mechanical processes happening within the rock mass. In particular, when considering the material's microstructure and the labyrinthine pore network, X-ray CT emerges as the most powerful NDT technique allowing real-time 3D characterization of the fingering patterns. The fast image acquisition and the high spatial resolution provided by the X-ray CT enable capturing the time-resolved volumes of the developing fluid interface in the pore space.

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MS10 / 461

**In-Situ Micro-CT Studies to Understand the Role of Salt Precipitation during CO<sub>2</sub> Storage in Saline Aquifers****Authors:** Puyan Bakhshi<sup>1</sup> ; Omid Shahrokhi<sup>1</sup> ; Susana Garcia<sup>1</sup> ; Mercedes Maroto-Valer<sup>1</sup><sup>1</sup> *Heriot-Watt University***Corresponding Authors:** m.maroto-valer@hw.ac.uk, s.garcia@hw.ac.uk, pb62@hw.ac.uk, o.shahrokhi@hw.ac.uk

CO<sub>2</sub> injection into underground geological formations, particularly saline aquifers, causes the removal of water by evaporation into the CO<sub>2</sub>-rich phase. This process triggers salt nucleation and precipitation inside the pores, and therefore, alters the petrophysical properties of the formation rock.

In the context of CO<sub>2</sub> storage, several experimental studies have been conducted at pore and core scales to investigate salt precipitation. While micromodel experiments have provided a 2D insight into salt precipitates at the pore scale [1, 2], core flooding tests have been extensively employed to mimic this process in natural porous media. These core-scale experiments have mostly been used to monitor the petrophysical alterations due to salt precipitation during CO<sub>2</sub> injection and have reported porosity and absolute permeability reductions [3, 4]. The advent of X-ray microtomography (micro-CT) has facilitated the rapid, non-destructive, in-situ 3D imaging of rock-fluid systems. This technique provides a comprehensive pore-scale characterisation of rock samples down to microns, as well as the distribution, morphologies, and characteristics of the occupying fluids. However, using micro-CT scanning for monitoring such a flow process is challenging due to high-pressure/high-temperature (HPHT) subsurface conditions, which need to be replicated because of the dramatic impact of such conditions on fluid properties and fluid/rock interactions.

In this work, we aim to investigate salt precipitation induced by CO<sub>2</sub> injection in natural porous media by providing direct, 3D pore-scale evidence using in-situ HPHT micro-CT imaging. Although this technique has been extensively used to study many CO<sub>2</sub> storage related topics, it has rarely been utilised for imaging the potential petrophysical alterations due to salt precipitation during storage operations. Accordingly, we have designed and developed a unique HPHT micro-CT core flooding system, which is an excellent tool for providing valuable 3D information of flow processes at realistic subsurface conditions. The system consists mainly of two parts: (1) the micro-CT instrument itself capable of performing high-resolution scans down to a nominal pixel size of 3 microns; and (2) the HPHT flooding system, the main part of which is an X-ray transparent flow cell, capable of withstanding elevated pressures and temperatures to provide the conditions of typical deep saline aquifers.

Despite the numerous experimental studies published in this area, the impact of salt precipitation on the flow paths of the injected CO<sub>2</sub> and the potential alteration of its effective permeability is still a subject of discussion. Hence, the main objective here is to investigate the nucleation, precipitation, and dry-out mechanisms, as well as the extent of injectivity reduction at the pore scale. Accordingly, micro-CT scanning of the drying process of a brine-saturated rock sample (diameter ≈ 5 mm) by dry gas injection is conducted. The analysis of the CT images taken before and after the experiments quantifies the precipitate particle sizes, the extent of pore size alterations, and the pattern of precipitation. Moreover, this presentation explores different injection conditions mimic the potential of salt precipitation at different distances from the injection well and analyses the resulting patterns of such a process.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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**Poster + / 449**

## **In-situ real-time imaging to characterize spatially heterogeneous calcite dissolution rates at the nanoscale**

**Authors:** Gianlorenzo Bussetti<sup>1</sup> ; Lamberto Duo<sup>1</sup> ; Alberto Guadagnini<sup>1</sup> ; Chiara Recalcati<sup>1</sup> ; Monica Riva<sup>1</sup> ; Martina Siena<sup>1</sup>

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Carbonate dissolution processes are significant in environmental and industrial contexts. Development of proper modeling frameworks to tackle, e.g. aquifer contamination, geologic carbon sequestration, disposal of toxic waste or hydraulic fracturing of hydrocarbon reservoirs requires enhanced and detailed knowledge of mineral dissolution/precipitation reactions kinetics. Advanced measurement instruments such as Atomic Force Microscopy (AFM) and Vertical Scanning Interferometry (VSI) have been recently employed to directly observe mechanisms involved in these reactions at the fluid-solid contact. Such studies have documented that there are several sources of variability that may affect the dissolution process at the microscopic level across mineral-fluid interfaces. This, in turn, yields marked spatial heterogeneities of reaction rates. A change of perspective towards an approach yielding quantification of reaction kinetics within a stochastic framework is of critical importance in this context. We employ modern geostatistical tools to characterize the spatial heterogeneity of reaction rate maps evaluated from a collection of in-situ and real time AFM observations of the surface topography of a millimeter-scale calcite sample subject to dissolution. Our aims include (1) the characterization of the statistical behavior of topography and dissolution rate data and their spatial increments; (2) the identification of an appropriate interpretive statistical model; and (3) a quantitative evaluation of the temporal evolution of the spatial heterogeneity of reaction kinetics.

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**Poster + / 471**

## **Incompressible Smoothed Particle Hydrodynamics as a tool for modelling electrolyte distribution in Gas Diffusion Electrodes**

**Authors:** Thorben Mager<sup>1</sup> ; Manuel Hopp-Hirschler<sup>1</sup> ; Ulrich Niekem<sup>1</sup>

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In electrochemical synthesis processes like chlor-alkali electrolysis with oxygen-depolarized-cathodes, porous Gas Diffusion Electrodes (GDE) have to ensure the intimate contact between the silver catalyst, the gaseous reactants and the liquid electrolyte. In the manufacturing process of the electrodes non-wetting Polytetrafluoroethylene (PTFE) is added to change the wettability of this electrodes. Electrochemical experiments showed a strong dependence of the PTFE content on the performance of such electrodes [1]. Understanding the electrolyte distribution in GDE enables the possibility for further improvements of the process.

To model the mixed-wet behaviour, the Lagrangian Smoothed Particle Hydrodynamics Method (SPH) can be used to solve flow-problems on the microscale. Recently, Kunz et al. showed the capability of the SPH-code SiPER (Smoothed Particle Hydrodynamics in Process Engineering) to model these structures based on FIB-SEM images [2]. We present simulation results based on dynamic SPH simulations of the electrolyte imbibition process to estimate the pore entry pressure dependent on wettability effects at the fluid-fluid-solid-interfaces resulting from the PTFE-distribution, external pressure gradients and flow configuration. However, modelling of representative volumes is still challenging due to the high computational demand.

As an outlook, we will present several ways to model larger structures of the GDE. Beside the improvement of scalability and the numerical methods for the SPH-method, the separate treatment of single pores, to use the corresponding entry pressure as an input for a Pore Network Model (PNM), can be used to model the electrolyte distribution on larger parts of the porous structure.

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MS9 / 754

## Influence of intermittency effects on anomalous transport in single- and multi-phase flow in porous media

**Author:** Zoë Penko<sup>1</sup>

**Co-authors:** Yaofa Li<sup>2</sup>; Amirhosein Begmohammadi<sup>1</sup>; Diogo Bolster<sup>1</sup>; Kenneth Christensen<sup>3</sup>

<sup>1</sup> *University of Notre Dame*

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Multi-phase flow and transport in porous media is prevalent in a wide range of challenging fluid mechanics problems in sustainability, energy, and the environment. Accurate prediction of the displacement and interaction of such flows is vital in addressing these problems, particularly the small- or pore-scale study of the flow's spatial and temporal evolution, which can impact flow behavior at system scales in a nontrivial manner. Intermittency is a phenomenon currently observed in numerical and experimental studies of single-phase flow, but the case of multi-phase flow has yet to receive much study in this regard due to challenges faced in both simulations and experiments. Due to strong nonlinearities and nonlocalities, a comprehensive understanding of multi-phase flow at very small scales is necessary in the development of accurate upscaled system-scale prediction models. We present results from a coordinated numerical and experimental study of intermittency effects over a range of viscous and inertial flow regimes in single- and multi-phase flows in 2D porous media micromodels to quantify Lagrangian flow statistics. The applicability of different modeling frameworks such as the correlated-continuous time random walk is tested by studying statistics of particle trajectories obtained by experimental particle tracking velocimetry measurements and numerical particle tracking in Lattice Boltzmann simulations.

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MS25 / 344

## Initial estimation of field-scale macropore parameters for use in dual-permeability models

**Author:** Carlos Alberto Faúndez Urbina<sup>1</sup>

**Co-authors:** Jarbas Honorio de Miranda<sup>2</sup>; Martinus Th. van Genuchten<sup>3</sup>; Bruna Marques de Queiroz<sup>2</sup>

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Macropore flow in near-surface soils can increase contamination risk of underlying water resources by agrochemicals. Macropore flow is commonly simulated using dual-permeability models (DPMs) involving separate equations for flow in the soil matrix and the macropores, which then are coupled using a lateral mass transfer equation. A large number of parameters and difficulty of measuring them independently under field conditions make routine application of DPMs a challenge. An additional difficulty is that soil profiles commonly show very heterogeneous distributions of macropores versus depth. A methodology is proposed to use disk infiltrometer data to obtain estimates of the two main macropore flow parameters: the relative macroporosity ( $w_f$ ) and the matrix domain characteristic length, generally associated with soil aggregates ( $dag$ ). Disk infiltrometry is used to obtain  $w_f$  estimates assuming the presence of cylindrical macropores. We expanded the approach for other macropore-matrix geometries (e.g., rectangular slabs) by invoking a transformation factor ( $\zeta$ ). Estimates of  $\zeta$  were obtained using pore-scale modeling by comparing non-cylindrical macropores' values against those having cylindrical shapes. Values of  $\zeta$  accounted for differences in macropore/matrix configurations and water flow rates. Remarkably, values of  $\zeta$  were found to be constant (equal to 1.5) for different macropore/matrix configurations.

The proposed methodology can be applied to different cross-sections in a soil profile, which would account for natural variations in  $w_f$  versus depth. Because  $w_f$  and  $dag$  are geometrically related, both parameters could be obtained simultaneously. The approach was improved by automated calibration using HYDRUS 2D/3D simulations in conjunction with disk infiltrometer data at zero pressure head.

Difficulties in the automated calibration were resolved using a meta-model for HYDRUS 2D/3D as generated in R script. The meta-model accounted for vertical heterogeneity in the macropore number using a general function with only four parameters: the value of  $wf$  at the soil surface ( $wfs$ ), the effective macropore radius, the maximum depth of macropores, and the shape parameter of the  $wf$  curve. The meta-model computed variations in  $wf$  and  $dag$  versus depth, thereby reducing the number of HYDRUS 2D/3D parameters for calibration. We show how the meta-model parameters can be obtained directly from infiltrometer data by illustrating an example for field conditions. A complete parametrization of the HYDRUS 2D/3D matrix and macropore parameters resulted from the data, and previous studies, as updated by automated calibration. Only  $wfs$  needed calibration, leading to a value about 3.5 times higher than its initial measurement (the Nash-Sutcliffe coefficient was 0.88). We could further relate several macropore parameters to  $wfs$  during calibration using physical or mathematical relationships. A good match can be obtained by either increasing  $wfs$  or the saturated hydraulic conductivity of the macropore domain. Future improvements may be possible by including additional information in the objective function, such as changes in storage water. Such changes could be estimated using non-destructive geophysical methodologies, such as ground-penetrating radar. Our study leading to initial point estimates of  $wf$  and  $dag$  should improve regional risk assessment studies where data for calibration are scarce and/or detailed plot studies are necessary to estimate macropore flow parameters

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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MS25 / 690

## Injectivity Decline by Nanoparticles in High Permeability Sandstone Rock

**Authors:** Ali Fadili<sup>1</sup> ; Ali Murtaza<sup>None</sup> ; Pacelli Zitha<sup>2</sup> ; Paul van den Hoek<sup>None</sup>

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Water injection and production is key to many industrial applications including hydrocarbon recovery, geothermal energy exploitation and ground water resource management. To comply with water quality requirements and environmental regulations, water is thoroughly treated and filtered before injection into the subsurface. Even after such extensive treatment, sub-micron solid particles remain suspended in the water. During injection, these particles are transported in the water and filtered by the porous structure, eventually plugging the formation and resulting in significant injectivity decline or even the clogging of the formation.

Injectivity decline studies reported in the literature thus far have focused on the filtration of particles in the micron range, especially from 1 to 5 microns. They have established is that severe injectivity decline arises from internal filtration and, after a certain transition time, the formation of an external filter. Attempts to apply this physical concept to the injectivity decline due the retention of nano-sized particles have so far been fruitless due to a large extent to the lack reliable experimental data.



This experimental study aims to fill that gap.

We report very well controlled laboratory experiments where ultra-filtered injection water is mimicked by water with dispersed spherical silica nanoparticles of about 140 nm diameter. The stability of nanoparticle colloid is investigated by varying nanoparticle concentration, brine compositions and pH. Their apparent hydrodynamic size and zeta potential show a range of salinity and pH where nanoparticles remain dispersed and within the expected size range. Then, core-flood experiments were conducted on Bentheimer sandstone. Pressure drop measurements along the core and influent/effluent analysis were used to analyse the transport and retention of nanoparticles in the cores. Experimental results show that stable injectivity is reached, along with a good propagation of the nanoparticles through the permeable core with no external filter cake formation, provided the pH and salinity of the injected fluid are kept within the stability range found in bulk. The injectivity decline show three different stages, which were matched using a 1D deep filtration model. The model includes three retention mechanisms: surface deposition, plugging and entrainment, and the simulations were found to be in very good agreement with the experimental results.

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MS16 / 121

## Inkjet printing lines onto thin, moving porous media - experiments

**Authors:** Vignesh Murali<sup>1</sup> ; Jos C.H. Zeegers<sup>1</sup> ; Anton A. Darhuber<sup>1</sup>

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Inkjet printing consists of the ejection and deposition of ink droplets on substrates that are moving underneath the printhead [1]. For printing on paper, water-based inks have been developed that are beneficial from an environmental standpoint. The printing of semi-infinite lines on moving paper substrates lead to a steady-state distribution of moisture and heat, which are a suitable way to study the interplay between heat and mass-transfer. Lateral wicking and evaporative mass loss are the dominant mass transfer mechanisms, while evaporative cooling reduces the temperature of paper by up to 6K.

Our goals were to develop an experimental setup and procedure to systematically measure the moisture content and temperature of paper as functions of the speed of the motion of the substrate and the frequency of droplet deposition. We use light transmission imaging and infrared thermography to measure the moisture content and temperature distributions, respectively. Our experimental setup consists of a sheet of paper, mounted 10 mm above an area light source and fastened onto a motorized translation stage. An inkjet printhead is placed a few mm above the paper surface. A CCD and an IR camera measure the transmitted intensity and the temperature of paper, respectively.

Besides conducting systematic experiments, we also developed a theoretical model for heat and mass transfer including evaporative cooling. The results of our simulations agree well with the measured data. Details of the model will be introduced in a separate presentation.

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Poster + / 122

## Inkjet printing lines onto thin, moving porous media - simulations

**Authors:** Gianmarco Venditti<sup>1</sup> ; Vignesh Murali<sup>1</sup> ; Anton A. Darhuber<sup>1</sup>

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Inkjet printing consists of the ejection and deposition of ink droplets on substrates that are moving underneath the printhead [1]. For printing on paper, water-based inks have been developed that are beneficial from an environmental standpoint. The printing of semi-infinite or long lines on moving paper substrates lead to a steady-state distribution of moisture and heat which are a suitable way to study the interplay between heat and mass-transfer. Lateral wicking and evaporative mass loss are the dominant mass transfer mechanisms, while evaporative cooling reduces the temperature of paper by up to 6K. Moreover, sorptive heating [1] needs to be considered, which can cause temperature increases above ambient on the order of 1K at the perimeter of the wet zone.

We developed a mathematical model coupling the Richards equation for moisture transport in unsaturated porous media with evaporative mass loss and heat transfer. The model is two-dimensional and only considers in-plane moisture transport, i.e. the short transient effects of moisture penetration in the thickness direction of the paper sheet are disregarded. We systematically varied the speed of motion of the printhead relative to the substrate and the frequency of droplet deposition to compare with the experimental data.

Our numerical model reproduces several key features of the experimental data. For example, the transverse widths of the moisture and temperature distributions, the maximum attained cooling amplitude and their scaling behavior as functions of substrate speed and droplet frequency are well captured by our model.

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V. Murali, J. C. H. Zeegers, A. A. Darhuber, *International Journal of Heat and Mass Transfer* 147, 118875 (2020). **Acceptance of Terms and Conditions:**

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MS1 / 710

## Insights from reactive percolation experiments on the geological storage of CO<sub>2</sub> in natural serpentinites

**Author:** Florian Osselin<sup>1</sup>

**Co-authors:** Michel Pichavant<sup>1</sup> ; Hugues Raimbourg<sup>1</sup> ; Marc Ulrich<sup>2</sup>

<sup>1</sup> *Institut des Sciences de la Terre d'Orléans*

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With global warming and increasing carbon dioxide concentrations in the atmosphere being probably one of the main scientific challenges of the XXIst century, the need to develop and implement Carbon Capture and Storage (CCS) technologies is more and more pressing. One possible solution which has been recently gaining momentum, is the storage of CO<sub>2</sub> as solid carbonates, which offers a much safer solution than the classical option of deep saline aquifers. Carbon dioxide mineralization can be proceeded in a variety of settings, but the potential of mafic and ultramafic formations (i.e. natural formations composed mostly of magnesium silicate minerals) is particularly appealing because of the large storage capacities (e.g. 77000 GtCO<sub>2</sub> in Oman ophiolites (Kelemen & Matter, 2008), even more if we consider the ultramafic content of the oceanic lithosphere), as well as the relatively short mineralization time (several years (Pogge Von Strandmann 2019)). When a carbonate rich fluid percolates in an ultramafic formation, the primary minerals dissolve, releasing their Mg<sup>2+</sup>, and potentially Ca<sup>2+</sup> in solution triggering the precipitation of Mg-carbonates (Power 2013). Moreover, as these formations are commonly rich in reduced iron (Fe<sup>2+</sup>), the high temperature percolation of water can also trigger the oxidation of ferrous iron to ferric and the concomitant reduction of water to H<sub>2</sub> (Klein 2013). This phenomenon which is commonly observed in nature (Charlou 2010) could also be leveraged to double the carbon dioxide sequestration with a H<sub>2</sub> production scheme.

However preliminary experiments show that the precipitation of carbonates in the porosity has a potentially dramatic effect on the permeability and thus the injectivity. Moreover, precipitation of carbonates can also have a negative impact on the host rock reactivity by precipitating on the substrate surface and thus shield it from further attack from the injected fluid.

In this study, we present 2 result from flow-through carbonation experiments on natural serpentinites at respectively 160°C and 280°C. Results show that precipitation of carbonates is responsible for a dramatic drop of permeability due to the clogging of the main percolation path. We interpret the final mineral assemblage as the result of the competition between mineral kinetics and fluid velocity scaled by the Damköhler and Péclet numbers. The reduction of permeability is due to the fast kinetics of carbonates, which allow them to precipitate locally and clog rapidly main flow pathways. In light of these experiments, a successful development of carbon mineralization techniques needs to address the precipitation issue in order to prevent a premature and catastrophic loss of injectivity. Possible solutions are the control of carbonate nucleation and kinetics, targeted hydraulic fracturing or even the potential leveraging of reaction-induced fracturing and crystallization pressure where the precipitation of carbonates could generates stresses on the porous matrix high enough to fracture it and thus open new percolation paths.

#### **Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS19 / 741

## Insights into capillary pressure in the GDL of operating polymer electrolyte fuel cells

**Authors:** Adrian Mularczyk<sup>1</sup> ; Lin Qingyang<sup>2</sup> ; Daniel Niblett<sup>None</sup> ; Jens Eller<sup>1</sup>

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X-ray tomographic microscopy (XTM) has become a versatile tool for the analysis of the microstructure in fuel cells, lithium ion and redox flow batteries, as well as the transport processes therein. Advanced analysis tools like 3D interfacial curvature analysis have been developed to determine the capillary pressure in digital rock physics investigations [1] and were recently applied to ex-situ XTM imaging experiments of the droplet release cycle in polymer electrolyte fuel cells [2]. Within this presentation, we will give insights into the water cluster formation using operando XTM imaging at a frequency of 1 Hz from liquid water emergence at the catalyst layer – gas diffusion layer interface until liquid water breakthrough and droplet formation in the gas channel of the flow field. With the help of interfacial curvature analysis as well as volume of fluid simulations [3], it was possible to obtain information about the capillary pressure evolution in the water phase. We will explain the nuanced interactions of water volume and pressure evolution during the growth of the percolation network within the GDL and the droplet formation and comment on the observed distinct differences to ex-situ pressure evaluations.

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MS15 / 779

## Integrating Machine Learning into a Methodology for Early Detection of Wellbore Failure

**Author:** Edward Matteo<sup>1</sup>

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There are literally a few million boreholes in the continental US (both onshore and offshore) that include abandoned wells, production wells, and wells for underground hydrocarbon storage. Some

are vulnerable to potentially catastrophic loss of seal integrity, largely owing to progressive damage of the annular cement sheath. The Deepwater Horizon oil spill and the Aliso Canyon natural gas leak have elevated wellbore integrity to national attention; new regulations have begun to address the effects of, but not causes of, well failure. It is conjectured that damage within the annular cement between host rock and well casing, engineered as the main seal between biosphere and subsurface, is one of the main leakage pathways. One approach to helping solve this problem is to utilize existing operational datasets from monitored wellbores as a testbed for developing methodologies that can screen for early detection of damage and/or failure.

There are few publicly available datasets of wellbore deformation, damage, and leakage due to geological forces. One existing group of datasets includes wellbores for several underground hydrocarbon storage facilities consisting of storage caverns built in salt domes. In these datasets, histories of wellbore casing damage have been determined from measurements taken by multi-arm calipers over many years. The operators of these facilities have observed some patterns to these deformation histories based on knowledge of the geomechanics of these salt domes, but a full explanation of these events is incomplete. This group of datasets has been selected for use in a machine-learning study to evaluate, interpret, and predict patterns of casing damage.

In our research, we explore using data science and machine learning (ML) methods to predict when a well might be approaching a state of failed seal integrity over time. We use Subject Matter Expert (SME) information as well as statistical techniques including correlation and regression analysis to define the features for our ML models. Our time series prediction considers both next time-step modeling as well as longer term time-series forecasting by utilizing random forests (RFs) and deep neural networks (DNNs) as well as recurrent neural networks (RNNs) for the predictions. The RF models allow us to perform feature importance characterization, while DNNs, specifically convolutional DNNs, facilitate utilization of spatial information including depth and volumetric data. We will utilize these models to characterize and automate the identification of factors that put wellbores at risk, so as to be used as an early detection system for failure screening that outperforms existing analysis tools.

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Time Block C (18:00-21:00 CET) **References:**

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MS15 / 319

## **Integrating process-based reactive transport modeling and machine learning for surrogate model development: an application to electrokinetic remediation of contaminated groundwater**

**Authors:** Riccardo Sprocati<sup>1</sup> ; Massimo Rolle<sup>1</sup>

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Multiphysics reactive transport models are nowadays widely employed in subsurface porous media and are able to account for several fully coupled physical and biogeochemical processes. However, the increasing level of detail of such models comes at the price of an increased complexity which often leads to long runtimes. As a result, explorative and probabilistic analysis that require numerous model evaluations are hampered by the excessive simulation time required.

To overcome this limitation, we show that it is possible to develop machine learning surrogate models which are able to predict the evolution of complex subsurface remediation systems using as

training data a limited number of process-based reactive transport simulations [1].

We focus on an application of electrokinetic enhanced bioremediation (EK-Bio), which aims at the removal of chlorinated solvents in low-permeability porous media. The modeling of this in situ remediation technology is challenging as requires the solution of coupled physical, electrostatic, chemical and biological processes. We developed a process-based, multicomponent reactive transport model of EK-Bio using the code NP-Phreeqc-EK [2], which can simulate the key mechanisms of electrokinetic flow and transport in multidimensional domains. The model accounts for electromigration and electroosmosis, Coulombic interactions, interphase mass-transfer, equilibrium and kinetically controlled reactions, including contaminant degradation and biomass dynamics [3].

The machine learning surrogate model was developed with a response surface approach using an approximation function based on an artificial neural network with a stack of multi-layer perceptrons. The surrogate model uses as inputs for the training the outputs of multiple runs of the process-based model, defined according to a design of experiments procedure. Subsequently, the surrogate model was trained with randomized cross-validation of hyperparameters. Comparing the surrogate model performances on a test set, the neural network demonstrated excellent prediction and generalization performances on all output variables. The developed surrogate allowed us to perform computationally efficient model exploration, global sensitivity analysis, and probabilistic uncertainty quantification.

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[1] Sprocati, R., & Rolle, M. (2020). Integrating process-based reactive transport modeling and machine learning for electrokinetic remediation of contaminated groundwater. In preparation.

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MS15 / 617

## Inter-well Connectivity Analysis and Productivity Prediction Based on Intelligent Connectivity Model

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Artificial neural networks (ANNs) are well known for its strong learning ability and have been widely used in the petroleum industry, such as history matching, production optimization and productivity forecast. However, ANNs are also a typical kind of “black box” models for their weakness in the model interpretability, causing their results less reliable than those from other physics based models. This paper proposes an integrated model named intelligent connectivity model (ICM), which incorporates ANNs with the material balance equation within a machine learning (ML) framework. ICM is a modular model, and each module keeps correspondence with each item in the material balance equation, improving the model transparency and generalization capability significantly. The results of simulation experiments show that ICM enables to generate comparable prediction results and provide more reasonable characterizations on inter-well connectivity than the classical physical model, and meanwhile ICM is more computationally efficient.

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MS24 / 352

## Interaction Problems between Fluids and Poro-Elastic Media - Applications in Life Sciences

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The urgent need for a better quantitative understanding of physiological processes in cells, tissues and the whole body is particularly evident in the current pandemic, in which the SARS-CoV2 virus is upsetting vital processes in the infected individuals. The damages of the virus at the cellular level, initially mainly in the lung, are causing inflammation that can get disordered and lead to a life-threatening breakdown of the organ system. An analysis of the processes involved in the infection and the reaction of the immune system shows that their influence on the structure and the biophysical and biochemical properties of the epithelial layers separating compartments in the body, in particular of the endothelium of the blood vessels is decisive. These interfaces determine the course of exchange processes and the vital reactions in the whole organism. Epithelial cell layers are regulators of barrier functions, controlling the transitions between different compartments, the exchange of chemical substances, of ions, of fluids, of cells. They are track switches of signalling and regulators coupling processes in different compartments. On cellular level, membranes and envelopes are playing a similar role, changing their permeability depending on the processes.

Mathematical modelling and simulation of these processes profit a lot from ideas and contributions of Andro Mikelic to multiscale analysis and its applications to porous media, in particular also to poro-elastic media. This report is dedicated to my long-time friend and outstanding partner Andro. A crucial problem in modelling and simulation is the coupling of diffusion, transport and reactions in a free flow and a flow in a poro-elastic medium. Assume that the elastic medium can be modelled by a Biot-System and that in the epithelial layer can be replaced by the boundary surface of this medium. The question arises: What are the appropriate transmission conditions?

The transmission conditions could be derived in a former joint paper with Andro Mikelic for the pure fluid flow and without an intermediate layer, in case of rigid porous media and under periodicity assumptions, investigating carefully the scale limits. A derivation of the transmission conditions using multiscale techniques is missing in case of poro-elastic media.

We formulated phenomenological transmission condition in two model systems, developed for

- osmotic swelling of a cell, modelled as a poro-elastic Biot medium.
- modeling of the inflammation, the regulation of the endothelial permeability and the formation of plaques.

Both topics lead to free boundary problems. Simulation results will be presented.

This report is based on joint research with Maria Neuss-Radu, Valeria Malieva, Telma Silva, Adelia Sequeira, Yifan Yang.

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Poster + / 329

## Interaction of Nanoparticles and Surfactant in Controlling Foam Stability

**Authors:** Mohammad Javad Shojaei<sup>1</sup>; Yves Méheust<sup>2</sup>; Abdulkadir Osman<sup>3</sup>; Paul Grassia<sup>4</sup>; Nima Shokri<sup>5</sup>

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Stability of foam in the presence of hydrocarbons is a crucial factor in the success of its use in various applications in porous media, such as soil remediation and enhanced oil recovery. (EOR). In this study, we investigate the effect of surfactants with different charges (anionic, cationic, and non-ionic) on foam stability in the presence of charge-stabilized silica (SiO<sub>2</sub>) nanoparticles. Toward this aim, a comprehensive series of experiments on a Hele-Shaw cell and a foam column is conducted at bubble and bulk-scale respectively, that is, investigating phenomenologies of foam coarsening separately by gas diffusion and gravitational drainage. Our results show nanoparticles, despite their ability to position themselves at liquid-gas interfaces and thus limit the resulting surface tension coefficient, do not necessarily have a positive effect on foam stability; the nature and magnitude of this effect depends strongly on the nature of the surfactant, its concentration and the concentration of nanoparticles. Both results from bubble-scale and the bulk-scale experiments suggest that compatibility experiments are pre-requisite to foam stability analysis to test the compatibility between surfactants and nanoparticles.

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MS25 / 791

## Intermediate-scale testing of a spatially distributed sensing technology for monitoring gas emission from soils as applied to climate change

**Authors:** Ana Ilie<sup>1</sup>; Tissa Illangasekare<sup>None</sup>; Kenichi Soga<sup>2</sup>; Richard Whalley<sup>3</sup>; Andrew Trautz<sup>1</sup>; Abdullah Cihan<sup>4</sup>



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The current understanding of the effects of soil management on carbon cycling and emissions of major greenhouse gases (e.g., H<sub>2</sub>O, CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O) is limited by the dearth of available sensing technologies that can make spatially distributed soil gas concentration measurements at the field and landscape-scales. It is important that these gas concentration data be furthermore be closely linked to high fidelity multi-scale soil structure and soil water content characterizations as these soil factors control the generation and transport of greenhouse gases. A combined laboratory and field study is in progress to develop and deploy a spatially distributed gas sensing technology with an embedded fiber-optics component for use in agricultural and the natural environments. This integrated sensing system will be tested under various soil, vegetation, and climatic conditions in a controlled laboratory setting using a specialized coupled micrometeorological wind tunnel and soil testbed facility at the ERDC synthetic environment for near-surface sensing and experimentation (SENSE). Prior to wind tunnel testing and subsequent field installation, a set of experiments were conducted in a three-dimensional intermediate-scale laboratory soil testbed. These experiments, performed under well specified and controlled boundary conditions, were designed to investigate the effects of soil heterogeneity on the spatial dynamics of soil moisture and subsequent gas migration pathway development. The soil testbed was packed with a heterogeneous configuration consisting of five uniform silica sands with the effective sieve numbers #70, #20/30, #16, #12/30, and #8. Spatial and temporal variations of soil moisture were monitored in situ with embedded soil moisture sensors. Gas concentrations were also measured within the soil profile and at the soil surface using a traversing fast-flame ionization detector. Methane was released from a set of ports located at the bottom of the soil test-bed to simulate a distributed natural/anthropogenic release. Various soil moisture dynamics scenarios expected in the field were simulated by fluctuating the water table and applying artificial precipitation using a rainmaker located above the soil testbed. The experimental data were used to validate a two-phase flow and gas migration model and demonstrate the importance of monitoring the soil moisture dynamics to properly/accurately interpreting gas concentration measurements within the soil profile and at the land-atmospheric interface.

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MS17 / 353

## Introduction of Anisotropic Heat Transfer Coefficient

**Authors:** Hermes Scandelli<sup>None</sup> ; Azita Ahmadi<sup>1</sup> ; Shaolin Liu<sup>None</sup> ; Jean Lachaud<sup>2</sup>

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This presentation addresses heat transfer in porous media with the assumption of local thermal non equilibrium (LTNE). The macroscopic description makes use of a two-equation model featuring a heat transfer coefficient between the solid and fluid phases. This coefficient can be determined from direct pore-scale numerical simulations by computing the ratio of the heat flux at the solid-fluid interface to the difference of the average temperatures [1]. When dealing with periodic materials, the resolution of the closure problems [2] obtained when using the volume averaging method can be considered for its evaluation. Both methods are widely used in the literature, but to our knowledge, no study has ever compared their predictions. For this reason, we have implemented both methods and applied them on basic periodic case where a creeping incompressible flow has been considered.

Results highlight two main facts. First, while the resolution of the closure problems provides a constant heat transfer coefficient, the method based on direct numerical simulations provides a time-varying coefficient that ends up to be equal to zero at steady-state. Special considerations are needed for a proper comparison of the two approaches. Second, as widely known, the heat transfer coefficient has shown to be a function of several parameters, mainly the Prandtl, Nusselt, and Biot numbers. The latter has been particularly investigated in this study by proposing a first analysis with homogeneous constant solid temperature and a second generic one with non-homogeneous and varying solid temperature.

Finally, the method based on direct numerical simulations is applied on a 3D CMT of Calcarb, a carbon fiber preform used as thermal protection in space vehicle heat shields. The results in terms of heat transfer coefficient are compared to experimental results obtained elsewhere [3].

The numerical framework developed during this study is made available in the Porous material Analysis

Toolbox based on OpenFoam (PATO) released Open Source by NASA [4] ([www.pato.ac](http://www.pato.ac)).

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## **Introduction of an Integrated Workflow for Optimal Well Placement Using Machine Learning Methods**

**Author:** Pouya Bakhtiarimanesh<sup>1</sup>

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Petroleum reservoir modeling procedure for production optimization is a complex problem and requires significant computational costs -rooted in reservoir simulation and post-processing. The advent of Artificial Intelligence -particularly supervised machine learning algorithms- in the petroleum industry is gained much popularity because of efficient functionality in terms of high dimensional data, computational cost and time. This study focuses on building an integrated workflow, in which the optimization variables are chosen and revised by the machine learning approaches and at the end, the methods' efficiencies and reliabilities will be compared, all together.

The Extreme Gradient Boosting (xGBoost) and Light Gradient Boosting Machine (LightGBM) algorithms are then used to build intelligent models. Because of the geological complexity, slight adjustments in well operational condition and location could yield dramatic changes in the objective function responses. In this study, the objective function is the net-present-value (NPV) for a specified operational life of the reservoir under study. To obtain the initial data set for models training, several numerical simulations were run by a self-developed simulation code, and based on them, the algorithms suggest the new appropriate location and condition for best response in each step. This effectively reduces the CPU time for the optimization tasks in the workflow. Then a new simulation starts upon the suggested values and at last, the predicted (from optimization algorithms) and simulated responses are compared. In this work there are three case studies: I) a homogeneous reservoir with just one production well, II) a heterogeneous channelized reservoir with just one production well, III) a heterogeneous channelized reservoir waterflood flooding.

In the first scenario, both algorithms show satisfying predictions and the optimum location of single well was selected correctly (R-squared of 0.943 and 0.999 for LightGBM and xGBoost, respectively). As a sub-result, the LightGBM algorithm can find this point sooner than xGBoost algorithm. In scenario II, the LightGBM and xGBoost show a similar response. Both methods reveal reliable results in the third scenario. Furthermore, the number of required simulations runs for LightGBM is slightly less to that for the xGBoost model.

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MS6-B / 649

## Inverse modeling of transient three-dimensional core-scale two-phase flows

**Authors:** andrea manzoni<sup>None</sup> ; Aronne Dell'Oca<sup>1</sup> ; Martina Siena<sup>2</sup> ; Alberto Guadagnini<sup>2</sup>

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We consider transient three-dimensional (3D) two-phase (oil and water) flows, taking place at the core-scale. In this context, we aim at exploiting the full information content associated with available information of (i) the 3D distribution of oil saturation and (ii) the overall pressure difference across the rock sample, to estimate the set of model parameters. We consider a continuum-scale description of the system behavior upon relying on the widely employed Brooks-Corey model for the

characterization of relative permeabilities and on the capillary pressure correlation introduced by Skjaeveland et al. (2000). To provide a transparent way of assessing the results of the inversion, we rely on a synthetic reference scenario. The latter is intended to mimic having at our disposal 3D and section-averaged distributions of (time-dependent) oil saturations of the kind that can be acquired during typical laboratory experiments. These are in turn corrupted by way of a random noise, to address the influence of experimental uncertainties. We focus on diverse scenarios encompassing imbibition and drainage conditions. We employ two population-based optimization algorithms, i.e., (i) the particle swarm optimization (PSO); and (ii) the differential evolution (DE), which enable one to effectively tackle the high-dimensionality parameters space (i.e., 12 dimensions in our setting) we consider. Model calibration results are of satisfactory quality for the majority of the tested scenarios, whereas the DE algorithm is associated with highest effectiveness.

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S.M. Skjaeveland; L.M. Siqveland; A. Kjosavik; W.L. Hammervold Thomas; G.A. Virnovsky (2000). Capillary Pressure Correlation for Mixed-Wet Reservoirs SPE Res Eval & Eng 3 (01): 60–67. <https://doi.org/10.2118/60900-PA> **Acceptance of Terms and Conditions:**

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MS4 / 761

## Investigating signatures of fracture evolution during the drying of clay-rich architected porous media

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**Co-author:** Laura Pyrak-Nolte<sup>1</sup>

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Chemo-mechanical coupling in rock is known to result in the generation of cracks from volumetric changes in minerals caused by hydration, carbonation, oxidation, precipitation, and mineral dissolution. Alterations to the microstructures and changes in the chemical and mechanical properties of materials resulting from these processes can produce different types of acoustic activity as fracturing occurs. Here we examine the acoustic emissions (AE) in polymineralic synthetic rock samples during dehydration to distinguish the signals that arise from the movement of fluid through a rock, debonding of clay structures and, the development, nucleation, growth, and coalescence of fractures.

The synthetic rock was composed of Ordinary Portland Cement (OPC), Ottawa sand, and montmorillonite clays. Four types of samples were made which consisted of (1) OPC only, (2) OPC and Ottawa Sand (mortar), (3) mortar and Montmorillonite clay, and (4) embedded bodies of Montmorillonite clay in mortar. Samples with clay contained either a random distribution of clay (sample 3) or an architected structure (e.g. clay balls, thin sheet, etc.) (sample 4). Unbounded geo-architected samples were also monitored during drying as moisture was removed from the medium, with intermittent 3D X-Ray Microscopy (Zeiss Xradia 510 Versa) to visualize the state of the system. The resolution of the X-ray images was 40 micrometers pixel edge length. The AE were recorded using a Mistras - Physical Acoustics (PAC) AE recording system with a 10MHz sampling frequency, threshold amplitude of 27dB, and PAC F15-alpha sensors which were connected to the AE system via preamplifiers and affixed to the sample with hot gorilla glue.

During drying fractures developed in the clay-rich medium as a result of shrinkage, which coalesced into intricate fracture networks with distinct features. No fractures were observed in the samples with no clay and the same background medium. The peak frequencies of AE events generated during

dehydration varied for the different samples. While the frequencies obtained for mortar samples occurred within a well-defined range (200-250 kHz.), a wider frequency band (50 – 300 kHz.) with lower frequencies was observed for the samples with distributed clay. The clay-rich specimens were found to produce a significantly large number of AE resulting from the development and growth of the microfracture networks. The AE data are supported by 3D X-Ray Microscopy data which shows the progression of dense fracture networks in the clay-rich samples during the period of dehydration.

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MS5 / 680

## Investigating the Effect of Enzymatically Induced Carbonate Precipitation on Hydraulic Properties

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Enzymatically Induced Carbonate Precipitation (EICP) can be used to engineer the properties of porous media in situ. By targeted precipitation within the pore space, EICP reduces porosity and, more importantly, also affects the hydraulic properties of the porous medium: its intrinsic permeability as well as its relative-permeability and capillary-pressure-saturation relations. While the change in porosity is a straight-forward result of the precipitated volume of carbonate minerals, the resulting changes of intrinsic and relative permeability as well as of capillary pressure are less trivial. However, those changes in REV-scale hydraulic properties are in the context of reservoir engineering of highest importance and interest. As a first step towards describing the impact of EICP on those properties, experiments are conducted on mineralizing sintered glass-bead columns and 2D micromodels using EICP under continuous pressure measurement. The precipitated mineral volume and its distribution are monitored by sophisticated imaging: within the column by micro X-ray computed tomography; within the micromodel by optical microscopy. The effects of the precipitates on the hydraulic properties is then approximated by conducting pore-network modeling on pore networks extracted from the obtained images. This allows for estimates of EICP-specific parameterizations for the effect of EICP on the hydraulic-properties based on the volume of precipitated carbonate.

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## Investigating the Influence of Non-Linear Interfacial Partitioning on Aqueous Film Forming Foam (AFFF) Transport and Retention in the Unsaturated Zone

**Author:** Masoud Arshadi<sup>1</sup>

**Co-authors:** Shuchi Liao<sup>2</sup>; Chen Liu<sup>2</sup>; Kurt D. Pennell<sup>2</sup>; Linda M. Abriola<sup>2</sup>

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The widespread use of aqueous film forming foam (AFFF) in fire suppression over many decades has resulted in contamination of industrial and military sites with per- and polyfluoroalkyl substances (PFAS). Due to their long-term persistence, environmental toxicity and bioaccumulation, PFAS have become emerging contaminants of critical concern, subjected to rapidly evolving regulations.

Knowledge of PFAS sorption and accumulation at the air–water interfaces is critical to understanding the transport and retention of these substances in subsurface environments. Furthermore, PFAS interfacial accumulation is associated with changes in surface tension, which can alter water phase flow and retention in unsaturated soils. This presentation provides an overview of coupled experimental and modeling research designed to explore the influence of interfacial accumulation and soil sorption processes on transport of selected PFAS in soils.

A matrix of batch and column experiments was undertaken with selected PFAS compounds, both individually and in mixtures, to explore their potential for soil sorption and retention at air-water interfaces. Experimental results reveal that PFAS sorption is non-linear, conforming to a Freundlich isotherm and that accumulation at the air-water interface is well-described by a Langmuir-Szyszkowski expression. Significant reductions in air-water interfacial tension were observed for concentrated PFAS solutions and AFFF formulations. These experiments also demonstrate the competitive soil sorption and air-water adsorption behavior of the select PFAS when present as a multicomponent mixture.

A variable saturation flow and transport model, HYDRUS, was modified to incorporate experimentally derived competitive partitioning relations and used to explore the influence of interfacial adsorption processes on PFAS transport and fate. A modification was made to HYDRUS to introduce compositional dependence (i.e., PFAS concentration dependence) of interfacial tension into the water flow solver. The HYDRUS code was also modified to improve the solute mass balance conservation for nonlinear partitioning relationships.

The modified model was used to simulate the field-scale transport, and retention of AFFF in the vadose zone under various realistic spill scenarios. Simulations reveal the potential effects of surface tension reduction on aqueous phase redistribution and PFAS migration in the soil profile, as well as the significance of nonlinear adsorption processes. In addition, simulations suggest that use of linear partitioning relations to represent interface accumulation could lead to significant overestimation of predicted mass retention. These findings demonstrate the potential influence of PFAS on unsaturated water flow and solute transport in soils and presents a methodology to couple these processes in a predictive modeling tool.

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MS3 / 607

## Investigation of Emulsion Flow in Microfluidic Fracture with Varying Aperture

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Emulsions flow in porous media has been found to play an important role in hydrocarbon recovery, especially in enhanced oil recovery (EOR) for conformance control in shale oil recovery where mixed oil and water flow through fractures. However, the mechanisms ruling emulsions flow remain elusive with studies mostly limited to empirical correlations. Recent development of microfluidic technologies allows direct visualization of fluid behaviors at pore-scale, but most studies of emulsions flow using microfluidic chips focus on straight channels or the behaviors of single droplets. In order to reveal the underlying mechanisms of emulsion flow in porous media, it is still required to study a more realistic scenario: the flow of sequential droplets in a flow channel with varying aperture.

We conduct emulsion flow experiments in a 3D printed transparent model that integrates an emulsion generator and a main flow channel. The emulsion generator consists of a T-junction to generate droplets of monodispersed size while to control dispersed phase flow rate, and a second T-junction downstream to regulate the continuous phase flow, which allows us to independently control three variables of emulsion flow: dispersed phase injection rate ( $Q_d$ ), droplet size ( $d$ ), and total emulsion flow rate ( $Q$ ). Downstream of the emulsion generator is the main flow channel, which consists of 100 'pore-throat' microstructures where the 'pore' and 'throat' are the maximum (0.8 mm) and minimum (0.2 mm) of fractures aperture. The pressure drop ( $\Delta P$ ) along the main flow channel is monitored.

Two regimes of emulsion flow through the fracture with varying aperture is identified. At low capillary number ( $Ca$ ), capillary pressure dominates and Darcy's law completely fails.  $\Delta P$  is determined by the number of droplets retaining in the main channel. At large  $Ca$ , viscous effects dominate over the capillary effects, and  $\Delta P$  approximates the value predicted by Darcy's law. As a consequence, many counter-intuitive behaviors are observed. For example, when  $Q_d$  and  $d$  are fixed,  $\Delta P$  becomes a non-monotonic function of  $Q$ . Specifically, when  $Q$  is very small, the system is in capillary regime, and  $\Delta P$  decreases with increasing  $Q$ , because the number of droplets retaining in the main flow channel decreases. However, when  $Q$  is very high, the system is in viscous regime, and  $\Delta P$  increases with increasing  $Q$  following Darcy's law.

We further establish a physics-based correlation to functionalize the pressure difference ( $\Delta P$ ) and thus the apparent viscosity by the three independent variables ( $Q_d$ ,  $d$ , and  $Q$ ). A phase diagram is summarized to demonstrate the transition between capillary regime and viscous regime. This work initiated a novel framework towards comprehensive understanding of emulsions flow in porous media.

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MS11 / 631

## Investigation of species transport in fractured media using 3D printed micromodels

**Author:** Alexandros Patsoukis Dimou<sup>1</sup>

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Carbonate rocks are multiscale systems where features in the order of few microns such as pores and throats interact with features on the order of a few millimetres, such as fractures and vugs. Fractures allow fluids to move at an extremely high speed through the reservoir and possibly leak out, which would undermine engineering efforts. We must thus be able to predict these fluid movements to ensure storage permanence of injected fluids. Recent advances in three-dimensional (3D) printing allows for cheap and fast manufacturing of complex porosity models, allowing investigation of specific flow processes in repeatable manner and enabling sensitivity analysis for small geometry alterations. These 3-D models can be printed with multiscale porosity structures that include large features such as fractures with smaller pores. Flow and transport in these multiscale structure can be modelled using high resolution pore-scale simulations, but these simulations are restricted to small domain (<10003 voxels). Darcy scale models with discrete fracture network can be applied, but they lack the exact representation of the fracture geometry. The Darcy-Brinkman-Stokes (DBS) equation gives a seamless transition between the Stokes and Darcy scales allowing us to solve the Navier stokes equation for the large features and Darcy's equation for the small features. Although the use of the DBS equation for calculation of flow field and permeability has been widely applied, the validity of the transport equation remains to be investigated. Here we present an experimental investigation of species transport during single phase flow in custom 3D printed multiscale micromodels with fractured geometries. Different scenarios are examined where the connectivity of the fractures as well as the fracture shapes and apertures vary and their impact during single phase flow in the matrix is presented. The experimental results are then compared to high-resolution pore scale modelling simulations, 2D depth averaged simulations, and 2D multiscale simulations. The results of this work can be used to benchmark multiscale-simulations solving the single-phase Darcy-Brinkman-Stokes equation.

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**Poster + / 536**

## **Investigation on multi-scale pore seepage model of shale gas reservoir considering diffusion and slippage effect**

**Author:** Lijuan Jiang<sup>None</sup>

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Shale gas reservoirs which are usually heterogeneous ones have a multiplicity mode of occurrence. A comprehensive understanding of the complex migration mechanism is prerequisite to fully comprehend the reservoir seepage. In this paper, the gas flow types are classified based on Knudsen number; the aperture distribution is introduced as the weight coefficient of the comprehensive constitutive equation. Then, the multi-scale pore time fractional order seepage model considering the influence of real gas effect, diffusion effect and slippage effect, is established. The reliability of the new model is verified using the existing experimental data presented in previous literature. Our results show that the new model can accurately capture all the mechanisms of gas migration, and well characterize the influence of structure heterogeneity and real gas effect. Moreover, analysis results also indicate the diffusion effect and slippage effect play a critical role in the multi-scale seepage happened in shale gas reservoir. In conclusion, the new model which considers the real gas effect, diffusion effect and slippage effect, can accurately calculate the apparent permeability, which is a key issue in the production dynamic analysis and productivity prediction of shale gas.

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MS1 / 103

## Lab-scale characterization of a shaly caprock for CO<sub>2</sub> storage: advancements and limitations

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The potential of CO<sub>2</sub> underground storage relies on the sealing efficiency of the overlaying caprock that acts as a geological barrier. Shales are extensively studied as potential caprock formations thanks to their favourable hydro-mechanical properties and their sealing capacity: low permeability, high sorption capacity, high swelling ability and high capillary entry pressure. The sealing capacity of a geomaterial is usually quantified based on its measured capillary entry-pressure, i.e. the max. pressure difference that may exist across the interface that separates two immiscible fluids before the non-wetting fluid penetrated the pore space.

The water retention properties of shales have been previously studied in either gas-water or oil-water systems, however, no results for CO<sub>2</sub>-water systems are reported to this day. In this work, the capillarity of a shaly caprock geomaterial is investigated with a series of break-through tests (meso-scale). Based on these results, the capillary pressure (P<sub>c</sub>) - saturation (S<sub>w</sub>) relations of CO<sub>2</sub> displacing water (drainage) and water rewetting (imbibition) are explored and modelled based on the basic principles of unsaturated soil mechanics. The final goal is to project the main findings of the work to possible implications for caprock integrity (entry-pressure) and sealing properties (permeability) for safe CO<sub>2</sub> storage. To this end, the transport properties of the material before and after CO<sub>2</sub> injection are assessed and compared to previous results. The impact of the boundary conditions (pressure and temperature) to the retention, transport and sealing properties of the caprock material are evaluated. The interpretation of the obtained results is supported by an additional series of injection tests, this time in the micro-scale, the kinematics of which are observed and measured locally with in-situ x-ray tomography.

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Time Block B (14:00-17:00 CET) **References:**

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Poster + / 439

## Laboratory scale investigation of CO<sub>2</sub> flow mechanisms across clay-rich caprock

**Author:** Iman Rahimzadeh Kivi<sup>1</sup>

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Carbon capture and geologic storage, mainly in deep saline aquifers, is extensively considered as an essential component of any strategy to achieve carbon neutrality and effectively mitigate climate change. At pressure and temperature conditions relevant to CO<sub>2</sub> storage in sedimentary formations, CO<sub>2</sub> is less dense than the resident brine and tends to float, threatening the long-term storage operations [1]. Therefore, successful deployment of geologic CO<sub>2</sub> storage relies on ensuring the sealing capacity of caprock overlying the host formation. Bringing together experimental methods and a numerical interpretation scheme, we aim at shedding light on the processes governing CO<sub>2</sub> intrusion and flow through low-permeability shaly caprock. We perform CO<sub>2</sub> injection experiments on Opalinus Clay samples retrieved from the Mont Terri underground rock laboratory in Switzerland. Two types of Opalinus Clay are examined: intact shaly specimen, representing an ideal caprock for CO<sub>2</sub> storage, and remolded shale, representing the potential shear zone in the caprock [2]. The latter is found to possess higher intrinsic permeability and lower capillary entry pressure than intact rock. We parameterize a two-phase flow model in deformable porous media using appropriate hydromechanical properties and replicate experimental observations. Simulation results highlight three concomitant flow mechanisms: molecular diffusion of CO<sub>2</sub>, bulk volumetric advection of CO<sub>2</sub>, and brine advection transporting dissolved CO<sub>2</sub>. The bulk CO<sub>2</sub> intrusion is confined to the lowermost portion of the specimen and remains unable to trigger an effective increase in the relative permeability of CO<sub>2</sub>. Therefore, advective CO<sub>2</sub> migration is minor. We conclude that rapid capillary breakthrough of CO<sub>2</sub> is unlikely to take place and compromise the sealing capacity of nonfractured caprock. The relatively slow diffusive flow appears to purely dominate leakage in the long term. Yet, diffusive CO<sub>2</sub> leakage may occur over geological time scales and have to be assessed in field-scale tests and through numerical simulations.

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MS8 / 440

## Lagrangian Intermittency in Colloid Transport Through Porous Media

**Authors:** Veronica Morales<sup>1</sup> ; Markus Holzner<sup>2</sup>

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We present a study of the characteristic time scales and Lagrangian intermittency of colloidal suspensions moving in porous media. The phenomenology of intermittency constitutes long periods of slow particle motion interrupted by brief bursts of high velocity. For particles of finite size and mass, we conjecture that intermittency is associated with the inexact velocity thresholds that define when particles are mobile or immobilized. Traditionally, transport models based on Colloid Filtration Theory smooth out small-scale Lagrangian intermittency that is key to understand transport processes under *unfavorable* conditions, during which particles spend substantial time near the surface of the filter medium. Using the concepts of *flying* and *diving* residence times above and below a given velocity magnitude threshold we infer the Lagrangian time distributions for colloid deposition and detachment, respectively. The analysis is obtained from over  $3 \times 10^4$  trajectories recorded with three-dimensional particle tracking velocimetry in a refractive index matched porous medium. We propose a definition for deposition rate in terms of exit-time statistics from flying events along each particle path. A similar definition for detachment rate presented in terms of exit-time statistics from diving events. This amounts to measuring the time it takes for a particle to get into or out from a state of low mobility. More generally, our study brings new information to the manner in which deposition and detachment rates are quantified based on Lagrangian residence time distributions rather than average values. Considering the variability in reaction rates for colloidal suspensions could resolve discrepancies between observations and predictive models of colloid transport and filtration.

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MS6-B / 368

## Lamellae Generation and Dynamics During Gas Invasion of a Porous Medium Occupied by a Surfactant Solution

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Foam is widely used in oil recovery operations to improve sweep efficiency, in gas storage and acidization operations, and to solve problems caused by either a thief zone or gravity override. Foam, which can be pre-formed and injected in the reservoir or produced in-situ through the pore space, fills the high permeability areas known as thief zones and divert the displacing fluid into the direction of trapped oil, reducing the relative permeability of gas and leading to a more stable displacement front. The efficiency of these processes largely depends on the generation and stability of the foam films (lamellae) residing in the pores.

The mobility of the injected gas is reduced when it's foamed; this reduction is attributed to the increase in the gas effective viscosity and the reduction in gas relative permeability. The lamellae formed create resistance against the gas flow, impeding its free motion inside the porous media. The lamellae population that composes the foam is direct related with surfactant concentration, and their flow and mobility are functions of the pore geometry and foam properties. However, the dynamics of foam formation in porous media is not fully understood due to its complexity.

The goal of this research is to understand the dynamic process of gas invading a two-dimensional porous media glass model occupied by a surfactant solution and forming foam. A microfluidic setup composed of glass micromodel, syringe pump, pressure transducer and microscope, was used to visualize the pore-scale displacement and correlate the evolution of lamellae formation during the injection process with pressure difference for different flow conditions through image processing.

The dynamics of lamellae formation and speed is reported and related to macroscopic flow behavior.

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MS9 / 403

## Lattice Boltzmann modeling of contact angle hysteresis in liquid drying in porous media

**Authors:** Feifei Qin<sup>1</sup> ; Jianlin Zhao<sup>2</sup> ; Qinjun Kang<sup>3</sup> ; Dominique Derome<sup>4</sup> ; Jan Carmeliet<sup>5</sup>

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Drying in porous media is a complicated multi-physical process including liquid/vapor multiphase flow, phase change and heat and vapor transport, occurring with the complex geometry of porous media. Contact angle hysteresis induced by surface roughness is shown to influence drying of liquid or colloidal droplet, resulting in a stick-slip drying mode and the formation of coffee ring after drying in constant contact radius mode. However, the influence of contact angle hysteresis on liquid drying in porous media still lacks exploration, either experimentally or numerically.

Lattice Boltzmann model (LBM) is an advanced numerical approach that can model phase change problems such as evaporation and boiling. In this paper, utilizing a geometric formulation scheme to prescribe contact angle, we present a contact angle hysteresis model within the framework of a two-phase pseudopotential LBM. First, we simulate droplets sitting on flat and curved surfaces, to validate the capability and accuracy of prescribing and automatically measuring contact angles over a large range. The proposed contact angle hysteresis model is further validated by modeling droplet drying on flat and curved surfaces. It is found that by considering contact angle hysteresis a stick-slip mode on both surfaces can be captured. Drying of two connected capillary tubes is studied, considering the influence of different contact angle hysteresis ranges on the evolution of liquid-vapor interface. The model is finally applied to study drying of a dual-porosity porous medium with/without considering contact angle hysteresis, where liquid configuration and drying rate are compared showing important differences. The proposed model is shown to be capable of dealing with different contact angle hysteresis ranges accurately, and of capturing the physical mechanisms during drying in different porous media.

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MS19 / 398

## Lattice Boltzmann simulation in the context of battery systems

**Author:** Martin Lautenschläger<sup>1</sup>

**Co-authors:** Julius Weinmiller<sup>1</sup> ; Timo Danner<sup>2</sup> ; Arnulf Latz<sup>3</sup>

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Simulations based on the Lattice Boltzmann method are a powerful and efficient tool for the investigation of mesoscopic processes that are hard to study experimentally. Such simulations have been used successfully to study redox flow batteries [1]. But they have rarely been used to study transport mechanisms in other battery systems [2,3]. In the present work, the wetting process during the electrolyte filling in the battery production is investigated by means of the flow of electrolyte through realistic three-dimensional porous battery electrodes. The electrode microstructures are generated using a sophisticated stochastic model [4] for the active material which is complemented by an additional binder phase. The focus of the study is on determining the capillary pressure-saturation relation during electrolyte intrusion and drainage. The main influencing factors investigated in the present work, are the porosity of the electrodes, the proportion of the binder phase as well as the wetting behavior of both the active material and the binder. Besides, also the effect of spatially non-resolved nanopores in the binder is studied using a homogenization approach. Lattice Boltzmann simulations with different multiphase flow methods, i.e. the Shan-Chen pseudopotential method [5] and the color gradient method [6], are conducted. Results from both methods are compared with each other. For validation purposes, they are also compared against results determined using the pore morphology method. The results from the present study are shown to agree well with results from the literature. They are especially useful for optimizing the electrolyte filling process which is a time-determining step in the battery production.

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Poster + / 40

## Lattice Boltzmann simulations of invasion in porous transport layer (PTL) at anode side of polymer electrolyte membrane (PEM) water electrolyser

**Authors:** Supriya Bhaskaran<sup>1</sup> ; Nicole Vorhauer<sup>2</sup> ; Vikranth Kumar Surasani<sup>3</sup>

**Co-authors:** Evangelos Tsotsas<sup>4</sup> ; Shubhani Paliwal<sup>5</sup> ; DEBASHIS PANDA ; Tanja Vidakovic-Koch<sup>6</sup>

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Among the demanding challenges of the 21st century, clean energy supply is still challenging to the scientific community to mitigate global warming. In this regard, transforming renewable energy into a stable and reliable fuel form by electrochemical methods is a promising technology. The polymer electrolyte membrane (PEM) water electrolysis is a key technology which uses water as feedstock for hydrogen production. The efficiency of PEM electrolyzers is mainly due to well-coupled kinetics of flow and reaction that occur inside the porous electrodes. The microstructure inside the anodic PTL plays a major role for favourable kinetics by facilitating counter-current transport of water and oxygen. In this study, we elucidate the transport mechanisms inside the PTL for invasion of oxygen using Lattice Boltzmann method (LBM). A multiphase and multicomponent LBM (Shan Chen LBM) [1] is applied based on BGK collision operator. LBM simulations are used in optimising the structural parameters of PTL (i.e. pore structure, pore connectivity, pore shape) for efficient operation of water electrolyser. As a first step, LBM simulation for titanium felt PTL is compared with experimental data from literature as well as pore network modelling (PNM), see Figure 1. The Capillary number (Ca) and Bond number (Bo) are used to study the competitiveness between the capillary and viscous forces and gravity for understanding the evolution of invasion patterns. Further, LBM simulations for imbibition and drainage phenomena inside the anodic PTL will be shown and discussed based on a titanium felt PTL.

Figure 1: LB simulation invasion patterns for titanium felt PTL, comparison with experimental results from literature [2] and PNM simulations [3].

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MS5 / 367

## Life in a tight spot: How bacteria move in porous media

**Authors:** Sujit Datta<sup>1</sup> ; Tapomoy Bhattacharjee<sup>2</sup> ; Daniel Amchin<sup>3</sup> ; Jenna Ott<sup>3</sup>

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Bacterial motility is central to processes in agriculture, the environment, and medicine. While motility is typically studied in bulk liquid or on flat surfaces, many bacterial habitats—e.g., soils, sediments, and biological gels/tissues—are complex porous media. Here, we use studies of *E. coli* in transparent

3D porous media to demonstrate how confinement in a heterogenous medium fundamentally alters motility. In particular, we show how the paradigm of run-and-tumble motility is dramatically altered by pore-scale confinement, both for cells performing undirected motion and those performing chemotaxis, directed motion in response to a chemical stimulus. Our porous media also enable precisely structured multi-cellular communities to be 3D printed. Using this capability, we show how spatial variations in the ability of cells to perform chemotaxis enable populations to autonomously stabilize large-scale perturbations in their overall morphology. Together, our work thus reveals new principles to predict and control the behavior of bacteria, and active matter in general, in complex environments.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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MS25 / 56

## Linearized Water and Air Flow in Porous Media

**Authors:** Shmulik P. Friedman<sup>1</sup> ; Gregory Communar<sup>1</sup> ; Ido Nitsan<sup>1</sup> ; Ilan Ben-Noah<sup>1</sup> ; Ben Cohen<sup>1</sup> ; Alon Gamliel<sup>None</sup>

<sup>1</sup> ARO

**Corresponding Authors:** along@volcani.agri.gov.il, ben.cohen7@mail.huji.ac.il, communar@agri.gov.il, vwsfried@agri.gov.il, ilan.bennoah@mail.huji.ac.il, idon@volcani.agri.gov.il

The hydraulic and air conductivity and the water retention of porous media are non-linear functions of the water (or air) content or capillary pressure (Van Genuchten, 1980; Vereecken et al., 1989, 1990; Assouline and Or, 2013), which results in non-linear water and air, single- and two-phase flow equations that usually preclude analytical and necessitate numerical solutions. If assuming exponential dependence of the hydraulic (Gardner, 1958) or air (Philip, 1998) conductivity on the capillary pressure, the steady flow equations can be linearized when described in terms of the matric flux potential (the integral of the conductivity over the capillary pressure). If assuming also linear dependence of the hydraulic (or air) conductivity on the water (or air) content, the unsteady flow equations are also linear. The two major advantages of linear flow equations are that they facilitate analytical solutions to a variety of flow problems and that the action of multiple water (or air) sources can be described by linearly superposing the solutions describing their decoupled actions.

In the lecture, we will describe briefly a few applications of linear water (or air) flow equations for describing steady and unsteady, forced, water (or air) injection into porous media at different geometries and boundary conditions, relevant for several agricultural and environmental circumstances. These include: 1. Coupled point (or line) source irrigation and localized root water uptake (Communar and Friedman, 2010), which serves the major principle of; 2. The freeware DIDAS program for Drip Irrigation Design and Scheduling (<https://app.agri.gov.il/didas>, Friedman et al., 2016); 3. Evaluating the role of water availability in determining the yield/plant population density relationship (Friedman, 2016); 4. A proposed method for determining the soil hydraulic properties based on periodic point source irrigation (Communar and Friedman, 2014); 5. Simultaneous water uptake from an on-surface water source and from a shallow water table (in also laterally confined lysimeters) (Friedman and Gamliel, 2019); 6. Single-phase, air flow bounds (Ben-Noah and Friedman, 2019) to two-phase, air-water flow in periodic air injection (Ben-Noah et al., 2020).

Overall, the solutions to the simplified, linear water and air flow equations, described reasonably well measured distributions of water and air contents (pressures) and fluxes in a wide range of water (and air) contents, making them constructive, practical tools for the design and assessment of irrigation and subsurface air injection operations.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS13 / 283

## Linking DFT and MD to simulate grand canonical ensemble: selectivity of binary mixtures in nanopores

**Authors:** Mariia Vaganova<sup>None</sup>; Irina Nesterova<sup>None</sup>; YURIY KANYGIN<sup>1</sup>; Andrey Kazennov<sup>None</sup>; Aleksey Khlyupin<sup>None</sup>

<sup>1</sup> *Moscow Institute of Physic and Technology*

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We present an approach linking molecular Density Functional Theory (DFT) and Molecular Dynamics (MD) to the study of inhomogeneous fluids behavior in the nanoporous media. It is aimed at describing composition, volumetric and transport properties of the fluid confined within a nanopore that is connected with bulk (macropore). This problem is of interest for unconventional hydrocarbon reservoirs development, geologic carbon sequestration, gas separation and other industrial applications.

While DFT has been shown to reproduce adsorption and density distribution of confined fluid well, it is not applicable to describe transport phenomena. MD simulation can be used to obtain both structural and dynamic properties, but it is computationally expensive (especially in the case of modeling a large “bulk+nanopore” system). We propose an approach, in which MD simulation is performed only for confined fluid, and its initial configuration is based on DFT calculation of the fluid composition in a nanopore under given conditions in bulk.

In this work, we apply the proposed approach to study binary mixtures of methane, ethane and carbon dioxide in slit-like nanopores with carbon walls. Previously we validated both DFT and MD molecular models independently on experimental isotherms for the studied mixtures in bulk. We consider filling the nanopores of different widths with the fluid mixture when increasing bulk pressure. Detailed understanding of these processes is important for the petroleum industry (in particular, for enhanced gas recovery using CO<sub>2</sub> injection).

For each mixture we provide the dependencies of adsorption selectivity on bulk pressure and pore size obtained by DFT along with corresponding MD equilibration results. Bulk fluid composition is also varied and its effect on selectivity is analyzed. We consider typical reservoir conditions:



pressures up to 30 MPa and temperatures up to 400 K. Filling the pores with a width of 1–5 nm is studied in detail since the structure of fluid density profile varies most significantly in this range. DFT calculations are also provided for pore widths up to 50 nm to cover pore size distribution of unconventional reservoirs and observe stabilization of selectivity in larger pores.

Equilibrium density profiles of each component obtained by DFT and MD are compared. Both theory and simulation reproduce the layering structure of a confined fluid well. We observe the formation of an equal number of adsorption layers and (in the pores wider than 1 nm) the bulk-like region with constant density in the center of the pore. With increasing bulk pressure capillary condensation occurs, while the mixture in bulk is still gaseous. This can be observed from the density profiles and is visualized in snapshots from MD simulation.

Thus, in this work we apply a combination of theoretical (DFT) and simulation (MD) approaches to study the behavior of confined binary mixtures in equilibrium with bulk. The presented approach can be used to provide essential information for optimal design of CO<sub>2</sub> EOR in unconventional reservoirs and CO<sub>2</sub> sequestration.

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MS25 / 410

## Linking processes, scales, and research communities to advance research on the most important porous medium we have: our Earth.

**Authors:** Jan Vanderborcht<sup>None</sup>; Martinus van Genuchten<sup>1</sup>

<sup>1</sup> *Federal University of Rio de Janeiro*

**Corresponding Authors:** rvangenuchten@hotmail.com, j.vanderborcht@fz-juelich.de

Harry Vereecken's career is built around the most important live-sustaining porous part of the Earth: the vadose zone, including soil. Understanding the processes in this medium and characterizing its properties is not only an intriguing scientific challenge, it is also vital for sustaining human societies. It is impossible to overrate the important functions of this porous medium and the services it provides. Its multitude of functions need to be understood holistically so that it can be managed and used productively and sustainably. Harry Vereecken's research contributes to this holistic understanding since it covers a wide range of topics. He investigated water flow and storage in the vadose zone, transport of nutrients and other chemicals, and their overall biogeochemical cycles. His interest went beyond a qualitative understanding of these processes by trying to quantify the many interacting processes and properties involved. Unfortunately, vadose zone and soil research is still hampered by a lack of experimental methods and techniques to investigate and observe processes as they take place in their undisturbed, natural state. Developing and applying process imaging methods at different scales is another important branch of his research. He investigated soil properties and processes at a large range of scales: from the small soil column scale to the field scale and up to the global scale. Harry made clear that up and downscaling is not only a technical mathematical problem but also a question of knowledge transfer between research communities that work at the different scales. Building bridges between research communities and organizing and setting up community initiatives such as the international soil modelling consortium and the TERENO network of terrestrial observatories is a unique contribution with major impact on scientific progress, not only in this specific domain of vadose zone and soil science, but very much also in other closely linked research domains.

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MS6-A / 396

## Long-term redistribution of residual gas due to non-convective transport

**Authors:** Yaxin Li<sup>1</sup> ; Sally Benson<sup>2</sup>

<sup>1</sup> *Stanford University*

<sup>2</sup> *Stanford University*

**Corresponding Authors:** yaxinl@stanford.edu, smbenson@stanford.edu

Global climate change due to high dependence on fossil fuel has necessitated the need to deploy decarbonization technologies. Carbon capture and storage (CCS), a technology that stores CO<sub>2</sub> permanently in the subsurface, is largely seen as necessary to reduce CO<sub>2</sub> emissions from large-scale industrial sources. As CCS technology has become commercially viable, recent years have witnessed a large expansion of CCS projects driven by innovative incentive mechanisms and sustainable government support. Although mitigating global warming is a long-term goal, current engineering methods for CCS projects are focused on short-term operational parameters, typically 20-30 years. While CO<sub>2</sub> is expected to remain securely trapped in the subsurface, the long-term fate of injected CO<sub>2</sub> over thousands of years has yet to be investigated.

An important trapping mechanism for injected CO<sub>2</sub> is residual trapping, where a large fraction of injected CO<sub>2</sub> is disconnected into ganglia trapped in the pore spaces by capillary forces. A widely accepted theory is that residual trapping is responsible for permanent entrapment, as the trapped CO<sub>2</sub> ganglia is assumed to remain immobile until they eventually dissolve into the reservoir brine. However, field observation that supports this theory is hardly available due to long time scales of dissolution. In previous studies, we have shown that the residually trapped CO<sub>2</sub> is thermodynamically unstable due to capillary heterogeneity. This instability induces Ostwald ripening among residually trapped CO<sub>2</sub>, thereby redistributing the gas phase across the system despite the gas phase remaining immobile. This redistribution causes residually trapped CO<sub>2</sub> to re-aggregate and potentially remobilize, undermining the long-term security of geological CO<sub>2</sub> storage.

In this study, we evaluate the thermodynamic stability of residually trapped CO<sub>2</sub> from a fundamental perspective. By analyzing the chemical potential of the residually trapped CO<sub>2</sub>, we identify that in addition to capillary heterogeneity, both hydrostatic pressure and geothermal gradients lead to thermodynamic instability of residually trapped CO<sub>2</sub>. These driving forces induce non-convective transport of dissolved CO<sub>2</sub> in the aqueous phase, thereby redistributing the residually trapped CO<sub>2</sub> throughout the system in different directions. The resulting non-convective transport is a combination of multiple mass transfer mechanisms, including molecular diffusion, sedimentation of solutes and the Soret effect.

Furthermore, we study the characteristics of the non-convective transport and the resulting redistribution of residually trapped CO<sub>2</sub> through numerical simulation. Results indicate that hydrostatic pressure dominates the redistribution of residually trapped CO<sub>2</sub> by inducing molecular diffusion of dissolved CO<sub>2</sub>. This diffusive flux is upward such that the gas phase depletes in the bottom and accumulates at the top under the seal. Geothermal gradients can somewhat mitigate this accumulation by reducing the CO<sub>2</sub> solubility gradient. This diffusive flux depletes residually trapped gas in a rate of 10<sup>5</sup> years / m approximately. Although the non-convective transport is slow, the residually trapped CO<sub>2</sub> accumulates under the seal inevitably in a shorter period. Re-aggregation and remobilization of residually trapped CO<sub>2</sub> under the seal is highly likely to occur, which will be characterized in our future study.

**Time Block Preference:**Time Block C (18:00-21:00 CET) **References:**

Li, Yaxin, Charlotte Garing, and Sally M. Benson. "A continuum-scale representation of Ostwald ripening in heterogeneous porous media." *Journal of Fluid Mechanics* 889 (2020).

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MS24 / 641

## Long-time shadow limit for a reaction-diffusion-ODE system

**Author:** Anna Marciniak-Czochra<sup>None</sup>

**Corresponding Author:** anna.marciniak@iwr.uni-heidelberg.de

This talk is devoted to a problem of model reduction for a class of reaction- diffusion-ODE systems. Such systems of equations arise, for example, in modeling of interactions between cellular processes and diffusing growth factors. Taking into account different time and space scales of the underlying processes leads to singularly perturbed problems. We focus on a shadow limit approximation for systems with the largest diffusion coefficient tending to infinity that is shown to preserve pattern formation mechanisms. We provide a proof of shadow limit in case of very long-time intervals, i.e., time intervals scaled with the diffusion coefficient and tending to infinity for diffusion tending to infinity. In addition to the convergence result, we provide error estimates in terms of a power of the inverse of the diffusion coefficient.

The talk is based on a joint work with Chris Kowall and Andro Mikelić

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Poster + / 370

## Lubricated hydrodynamic interactions between a hard spherical indenter and a poroelastic nanolayer

**Author:** Caroline Kopecz-Muller<sup>1</sup>

**Co-authors:** Vincent Bertin<sup>2</sup>; Marjan Abdorahim<sup>3</sup>; Yvette Tran<sup>4</sup>; Patrick Tabeling<sup>3</sup>; Elie Raphaël<sup>2</sup>; Thomas Salez<sup>5</sup>; Joshua McGraw<sup>2</sup>

<sup>1</sup> *Gulliver (ESPCI) and LOMA (U. Bordeaux)*

<sup>2</sup> *Gulliver (ESPCI)*

<sup>3</sup> *MMN (ESPCI)*

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Soft and porous materials are present in a variety of contexts, from pharmaceutical applications to fundamental physics of interfacial soft matter. In particular, an intermediate layer of a soft material, present between a liquid phase and a solid boundary, can induce remarkable changes in lubrication mechanics. The motion of colloidal particles above a nanoscale grafted polymer layer is just one example of this general problem. Describing the behaviour of a such a particle in this context – that is, adding the porosity of the nearby surface to the elasto-hydrodynamic coupling – represents a relatively unexplored field. Here, we establish theoretical models to make numerical simulations of the particle motion. Preliminary experiments of Surface Force Apparatus (SFA) on PNIPAM hydrogels samples will also be presented, and applications to Atomic Force Microscopy will be discussed. Taking care to separate various physical aspects and their contribution to the global mechanism, will help to validate the theoretical predictions. Contributions to a better understanding of colloidal motion mechanisms influenced by a porous media will be obtained.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

LEROY, S. & CHARLAIX, E. J. of Fluid Mechanics, 2011

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ZHANG, Z. et al. PRL, 2020 **Acceptance of Terms and Conditions:**

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MS10 / 210

## MATBOX, an Open-Source Microstructure Analysis Toolbox for Meshing, Generation, Segmentation, and Characterization of 3D Heterogenous Volumes

**Author:** Francois Usseglio-Viretta<sup>1</sup>

**Co-authors:** Prehit Patel<sup>2</sup>; Jeffery Allen<sup>3</sup>; Aashutosh Mistry<sup>4</sup>; Partha Mukherjee<sup>5</sup>; Kandler Smith<sup>6</sup>

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<sup>2</sup> University of Alabama in Huntsville

<sup>3</sup> National Renewable Energy Laboratory

<sup>4</sup> Argonne National Laboratory

<sup>5</sup> Purdue University

<sup>6</sup> National Renewable Energy Laborator

**Corresponding Authors:** francois.usseglioviretta@nrel.gov, jeffery.allen@nrel.gov, ppp0002@uah.edu, kandler.smith@nrel.gov, pmukherjee@purdue.edu, amistry@anl.gov

Battery performance is strongly correlated with electrode microstructural properties. To account for its impact, lithium-ion battery (LIB) models either abstract the microstructural heterogeneity of composite electrodes using effective macroscopic properties (macro- or meso- scale models) or directly solve the system of equations on the microstructure geometry or mesh (microstructure-scale models). Therefore, to be adequate, both families of models require information from the microstructure geometry, which can be provided by the numerical tool presented in this work.

MATBOX is a MATLAB open-source application [1] developed by NREL for performing various microstructure-related tasks including microstructure numerical generation, image filtering and microstructure segmentation, microstructure characterization and correlation, visualization, and microstructure meshing. MATBOX was originally developed for the analysis of LIB electrode microstructures; however, the algorithms provided by the toolbox are widely applicable to other heterogeneous materials. The toolbox provides a user-friendly experience thanks to a Graphical-User Interface, requires no coding by the user, and is well documented. This presentation will illustrate various MATBOX features for the characterization of a LIB electrode, including a fully automated Representative Volume Element (RVE) analysis, the numerical generation of complex 'virtual' microstructure, including dual-layer electrodes and carbon-binder additive phase, and the meshing of a complex NMC/graphite full cell microstructure suitable for 3D finite-element modeling. Other modules (segmentation, visualization, and correlation) will be briefly presented.

Thanks to its modular, open-source approach, MATBOX can easily incorporate third-party algorithms to eventually build a standard in the field that will benefit the whole scientific community. Effective diffusion coefficient [2], additive phase numerical generation [3], and meshing [4] third-party algorithms have been already integrated in the toolbox with more to come.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

- [1] F. Usseglio-Viretta et al., MATBOX: an open-source microstructure analysis toolbox for microstructure generation, segmentation, characterization, visualization, correlation, and meshing (2020) <https://github.nrel.gov/fussegli/Micro>
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- [3] Mistry, A., Smith, K. & Mukherjee, P. P. Secondary Phase Stochastics in Lithium-ion Battery Electrodes. *ACS Applied Materials & Interfaces* (2018) doi:10.1021/acsami.7b17771.
- [4] Q. Fang et al., Tetrahedral mesh generation from volumetric binary and grayscale images. 2009 *Ieee Int Symposium Biomed Imaging Nano Macro* 1142–1145 (2009) doi:10.1109/isbi.2009.5193259. **Acceptance of Terms and Conditions:**

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**Poster + / 452**

## MOFs based CH<sub>4</sub> Hydrate Formation and Self-Preservation

**Authors:** Jyoti Shanker Pandey<sup>1</sup> ; Qian Ouyang<sup>1</sup> ; Nicolas von Solms<sup>1</sup>

<sup>1</sup> *Technical University of Denmark*

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Metal-Organic Framework (MOFs) are functional crystalline porous material having an open metal site with organic linkers with a wide range of applications. Fundamental properties include a large surface area, the high degree of crystallinity. It is also known that MOFs are of low density and show high thermal stability. Their usage in gas hydrate field is unknown and has not been investigated previously.

In this study, we test different MOFs for their CH<sub>4</sub> hydrate storage capability as well as storage stability below 0°C for natural gas storage and transport. Experiments are performed under hydrate formation conditions using a high-pressure chamber. Multiple temperature cycles are performed to check the memory effect as well as improvement in hydrate storage capability in memory run. Results show enhanced hydrate formation rate in the presence of MOF. During the study, crystals are found to remain stable over multiple dissociations and formation cycles, indicating a long life cycle and reusability of MOF as a hydrate carrier. Details discussion will be provided during the presentation.

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MS15 / 564

## Machine learning prediction of Lennard-Jones fluid self-diffusion in pores

**Authors:** Calen Leverant<sup>None</sup> ; Jeffery Greathouse<sup>1</sup> ; Jacob Harvey<sup>1</sup> ; Todd Alam<sup>1</sup>

<sup>1</sup> Sandia National Laboratories

**Corresponding Authors:** jharve@sandia.gov, jagreat@sandia.gov, tmlam@sandia.gov, c.leverant@ufl.edu

Porous materials are widely used in industrial applications (e.g., catalysis and separations) and diffusion of liquids within these materials can often control performance. Self-diffusion coefficients are typically obtained from molecular dynamics (MD) simulations in which the forces and trajectories of particles are calculated via Newtonian physics for millions of time steps. While MD provides accurate diffusion coefficients and can be tailored to a variety of circumstances (e.g., diffusion in pores), it is computationally expensive and requires large systematic studies in order provide insight as to which molecular properties affect diffusion. To provide a quicker, more computationally efficient alternative, we trained a variety of machine learning algorithms from simple linear models to complex convolutional neural networks to predict the diffusion of Lennard-Jones particles in a variety of ideal pore shapes. During the feature selection process, extra consideration was given to select features that are easy to obtain and understand by non-experts. Not only can these machine learning algorithms accurately predict diffusion coefficients at a fraction of the computational cost of MD, but they provide the opportunity to study the important features that contribute to the diffusion coefficient values. Insights obtained from studying the feature importance of these models can provide further understanding to the diffusion in porous media and enhance the materials design process for future porous materials used in industrial processes.

This work is supported entirely by the Laboratory Directed Research and Development Program at Sandia National Laboratories. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in this article do not necessarily represent the views of the U.S. Department of Energy or the United States Government. SAND2021-1589 A

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MS7 / 514

## Macroscopic model for flow in exuding porous media

**Authors:** Didier Lasseux<sup>1</sup> ; Francisco J. Valdés-Parada<sup>2</sup> ; Jean-François Thovert<sup>3</sup> ; Valeri Mourzenko<sup>3</sup>

<sup>1</sup> CNRS - Univ. Bordeaux

<sup>2</sup> Universidad Autonoma Metropolitana-Iztapalapa

<sup>3</sup> CNRS - Univ. Poitiers

**Corresponding Authors:** didier.lasseux@u-bordeaux.fr, iqfv@xanum.uam.mx, thovert@ensma.fr, valeri.mourzenko@ensma.fr

Single-phase macroscopic flow in a rigid porous medium is traditionally described by classical Darcy's law which can be formally derived by upscaling the pore-scale flow equation in the creeping incompressible flow regime and the no-slip condition at the solid-fluid interfaces. However, there are many situations for which fluid release from the surface into the pores or, conversely, absorption from the pores into the solid through the interfaces may occur. To cite some but a few, this case is encountered in drying (Vu & Tsotsas, 2018) and pyrolysis (Mahmoudi et al., 2014) of porous materials, vapor bubble migration in ice due to temperature gradient (Shreve, 1967) or processes for which a chemical reaction in a porous material leads to a net production of fluid from the surface into the pores or, conversely, absorption from the pores into the solid through the interfaces. This translates into a local normal flux at the solid fluid-interface, featuring a generic problem which may be referred to as flow in exuding porous media. Although classical Darcy's law has been widely heuristically employed to describe this type of flow, the question remains on the physical relevance of such an assumption.

In this work, the upscaling of low Reynolds number incompressible Newtonian flow in a rigid homogeneous exuding porous medium is performed using a mixed volume averaging/adjoint method. The upscaled model shows that the macroscopic velocity is non-solenoidal despite incompressibility. Moreover, the macroscopic momentum equation involves a Darcy term with the classical intrinsic permeability tensor corrected by a vectorial term including an effective component related to the local fluid displacement induced by exuding effects and, in some special cases, a compensation to non-locality. The two effective coefficients are obtained from a single intrinsic ancillary (closure) problem (Lasseux et al., 2021). The relevance of the macroscopic model is illustrated in many different examples through comparison between pore-scale numerical simulations and the macroscopic model predictions, showing excellent agreement. The results of this work motivate further research about the influence of internal flow sources in transport phenomena in porous media.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

Lasseux, D., Valdés-Parada, F. J., Thovert, J.-F. & Mourzenko, V. 2021 Exuding porous media: deviations from Darcy's law. *Journal of Fluid Mechanics* 911, 10.1017/jfm.2020.1081.  
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## Magnetic Resonance Imaging of Fluid Compositions in CO<sub>2</sub> Displacement of Decane in Berea Sandstone

**Authors:** Armin Afrough<sup>1</sup> ; Laura B. Romero-Zerón<sup>2</sup> ; Mojtaba Shakerian<sup>2</sup> ; Caleb A. Bell<sup>2</sup> ; Florea Marica<sup>2</sup> ; Bruce J. Balcom<sup>2</sup>

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Volume changes on mixing can significantly affect the flow of non-ideal mixtures in porous materials. In the case of a significant excess volume, the law of conservation of volume, instead of mass, governs flow equations. Such profound thermodynamic effects affect the modeling of many multi-component fluid flow processes in porous materials. Despite theoretical advancements in this regard, in-situ experimental data is still very limited, especially in systems in which the effect of dispersion is significant. The carbon dioxide/decane mixture is a simple two-component system that can form miscible and immiscible phases and model such complex behavior.

We utilized magnetic resonance methods to study the flow of carbon dioxide/decane mixtures in Berea sandstone at conditions where dispersion and thermodynamics effects are significant. Conventional magnetic resonance instruments and methods cannot image fluids at high-pressures and quantitatively – without significant losses of short-lifetime signal components. We employed a high-pressure controlled-temperature environmental metallic sample holder with an integrated radiofrequency probe that permits experiments at up to 35 MPa and 80°C. MRI methods, including Centric Scan Single-Point Ramped Imaging with T1-Enhancement (SPRITE), T2-Mapping Spin-Echo Single Point Imaging (SE-SPI), and  $\pi$  Echo-Planar Imaging ( $\pi$ EPI), in addition to free induction decay and CPMG methods continuously monitored the flow process.

MRI methods imaged fluid compositions of the carbon dioxide/decane mixture during CO<sub>2</sub> injection into decane-saturated Berea sandstone core plugs. MRI methods and parameters employed in this work were precise enough to permit accurate evaluation of partial derivatives of composition with respect to time and position in miscible, 9 MPa, and immiscible, 6 MPa, conditions – both at 40°C. Temporal and spatial derivatives of composition were acquired with a smoothing spline interpolation and processed to compute compositional wave velocity, dispersion coefficient, and the advection-dispersion kernel. The correlation of wave velocity with composition revealed the movement of leading and trailing shocks in agreement with fluid displacement theories and thermodynamics of carbon dioxide/decane mixtures. Local minima of wave velocity coincided with the extremum of mixture's excess volume. Magnetic resonance relaxation provided information about the composition of fluids in close proximity of the rock surface, complementary to compositions acquired by MRI.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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Afrough, A., Shakerian, M., Zamiri, M. S., MacMillan, B., Marica, F., Newling, B., Romero-Zerón, Balcom, B. J. 2018. Magnetic-Resonance Imaging of High-Pressure Carbon Dioxide Displacement: Fluid/Surface Interaction and Fluid Behavior, *SPE Journal* 23 (03): 772-787. <https://doi.org/10.2118/189458-PA>.

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MS10 / 646

## Magnetic Resonance and Magnetic Resonance Imaging of Porous Media – Recent Developments

**Authors:** Armin Afrough<sup>1</sup> ; Bruce J. Balcom<sup>2</sup>

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Magnetic resonance presents an array of unparalleled opportunities in probing fluids in porous media. Magnetic resonance methods are nowadays routinely employed in well-logging, monitoring underground water resources, laboratory analysis, and industrial process and quality control. Despite these widespread applications, there are significant problems associated with the inability of traditional magnetic resonance methods in observing short-lived signals typically observed in porous media. The University of New Brunswick (UNB) MRI Research Centre developed new methodologies to address these shortcomings and consolidated magnetic resonance imaging (MRI) as an excellent tool for in situ studies of a wide variety of materials, including rocks, sediments, wood, concrete, composites, foods, and microporous materials.

Innovations of UNB MRI Research Centre exploit (1) free induction decay as a means of signal formation for detecting short-lived signals, (2) low magnetic field intensities to reduce the effects of magnetic susceptibility difference of matrix/fluids, (3) pure phase encoding to avoid artefacts arising from susceptibility effects, chemical shift, B<sub>0</sub> inhomogeneity and linewidth restriction on resolution, (4) the importance of information in the proximity of k-space origin on the quantitative quality of data, (5) non-magnetic metallic environmental sample holders with integrated radiofrequency probes, and (6) correcting gradient waveforms or their effect. These innovations permitted quantitative and in vivo imaging of a variety of processes by a combination of specialized software and hardware. Several new discoveries and some interesting observations relevant to porous media applications were facilitated by these developments in the past few years:

(A) Magnetic resonance methods directly measured gas pressure in microscale pores of methane gas hydrates in a pioneering work. In a methane hydrate-bearing sand pack with 2.8% residual water at 2 MPa and 4°C, the elevated pore gas pressure was measured to be 59 MPa. (B) New models proposed for magnetic resonance relaxation in multicomponent mixtures in porous media were matched to experimental data on CO<sub>2</sub>/decane mixtures in Berea sandstone at 40°C and 6 MPa and 9 MPa, for miscible and immiscible conditions, respectively. The density of decane in the pore-surface bound layer decreased during the miscible drainage of decane by CO<sub>2</sub>. In contrast, in immiscible displacement of decane by CO<sub>2</sub>, the pore-surface area wetted by decane monotonically decreased only at saturations smaller than the residual saturation – consistent with the development of noncontinuous wetting films on the pore surface. (C) We established that nonground eigenvalues of the diffusion-relaxation equation indeed contribute to the magnetic resonance relaxation signal of common porous media, contrary to common belief. This discovery permits direct pore size estimation from common T<sub>1</sub> and T<sub>2</sub> distribution measurements. (D) The new T<sub>1</sub>-T<sub>2</sub><sup>2</sup> method proposed as a 2D relaxation correlation experiment permits the detection of mobile and immobile <sup>1</sup>H in porous materials, especially in shales and concrete material with significant susceptibility effects.

The recent addition of a variable-field superconducting magnet to the UNB MRI Research Centre is expected to further help the development of new methods and applications in porous media.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

<https://doi.org/10.1016/j.marpetgeo.2020.104296>  
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<https://doi.org/10.2118/189458-PA>  
<https://doi.org/10.2118/186089-PA>  
<https://doi.org/10.1063/1.5013031>

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MS25 / 328

## Magnetic resonance imaging of water content and flow processes in natural soil using pulse sequences with ultrashort detection

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**Background:** Soil water processes take place partly on small scales and are prone to distortion by invasive methods. Therefore, non-invasive imaging techniques are mandatory for their analysis and subsequent improved understanding. Contrary to XCT, which is most sensitive to the structure of the solid matrix, MRI is well suited to monitor the liquid phase due to its sensitivity to the substance of interest: water. The contrast relies on the water content and the properties of the soil pore manifesting in changed NMR relaxation times. Therefore, MRI is highly convenient too for the imaging pore space properties in addition to the water content. Vice versa, reduced relaxation times of some milliseconds often counteract the imaging of water content when using conventional MRI pulse sequences. A way out are so-called pulse sequences with ultra-fast detection. The purpose of the present paper is to adapt and test such sequences for quantitative water imaging in natural soil.

**Methods:** All experiments were performed using a Bruker, vertical super wide bore scanner at 200 MHz resonance frequency, allowing the percolation and sampling of water during scans. After the determination of relaxation properties of several soil materials, we have compared conventional and ultra-fast detection MRI pulse sequences (MSSE, ZTE, and UTE) with respect to their convenience for quantitative imaging of water content. The quantification of water content was performed with soil core samples of sandy loam for water contents between  $\theta = 0.1$  and  $0.4 \text{ cm}^3/\text{cm}^3$ . Next, the sensitivity for T2 blurring artefacts was tested at a composite sample with sand, sandy loam and silt loam soils. Finally, the optimal pulse sequence was applied for the mapping of flow processes in a natural soil core from Selhausen test site.

**Results:** Sandy-loam soil has relaxation times of  $T_1 = 80 \text{ ms}$  and two  $T_2$  fractions with 3 and 20 ms. Therefore, the conventional MSSE sequence hid larger fractions of water. In contrast, Zero-echo time imaging (ZTE) allowed the quantitative mapping of water content at a resolution of 0.5 mm in 3D in about 30 minutes/scan. T2 blurring artefacts were best eliminated for ZTE by increasing bandwidth to 300 kHz. Combining all these results, we used ZTE for the monitoring of the transition from matrix flow to film flow in a wormhole occurring in a ponded infiltration experiment in a natural soil core above a critical infiltration rate of 3.6 cm/h.

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**Conclusions:** The issue of rapid relaxation in natural soil can be overcome by ultra-fast detection. Water content changes are reliably mappable and processes such as the transition from matrix to preferential flow is detectable.

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MS22 / 498

## Manufacturing of polycrystalline nickel-based superalloy membranes by directional coarsening through rolling and ageing

**Authors:** Christian Voelter<sup>1</sup> ; Joachim Rösler<sup>None</sup>

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By coarsening of the precipitation phase, bicontinuous  $\gamma/\gamma'$  networks can be formed in nickel-based superalloys. Either the matrix or precipitate phase is then dissolved by (electro)chemical extraction to receive a  $\gamma'$ - or  $\gamma$ -membrane. Previous studies show that in single-crystalline CMSX-4, both rafting and pure thermal ageing result in complete interconnection of the respective phases. This creates directional and non-directional structures from which  $\gamma$ - or  $\gamma'$ -membranes can be produced, depending on the extraction process. Recent publications investigate the development of superalloy membranes made from a polycrystalline nickel-based alloy by incoherent growth of precipitation particles. Good mechanical properties are achieved by the production of  $\gamma$ -membranes.

In this work, we show polycrystalline membranes with a directionally coarsened structure. With the help of separate mechanical and thermal treatment, a rafted structure similar to the directionally coarsened one in CMSX-4 is also formed in the polycrystalline alloy. In contrast to the uniaxial creep load during the production of directionally coarsened single-crystalline membranes, a directional rafted structure is formed here from originally cubic  $\gamma'$  precipitates by repeated rolling and ageing.

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Poster + / 115

## Mapping Land Use and Land Cover Changes in Gilan Province of Iran between 1975 and 2015: GIS and Remote Sensing Analyses

**Author:** Noushin Khazaei<sup>1</sup>

**Co-authors:** Ali Zahedi<sup>2</sup>; Nima Shokri<sup>3</sup>; Ralf Otterpohl<sup>2</sup>

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Assessing the land use and land cover change is crucial for sustainable natural resource management and understanding the changes in hydrologic processes and water cycle. In this study, we aim to quantify the land use and land cover changes in Gilan province of Iran between 1975 to 2015 using Landsat 2 MSS and Landsat 8 OLI/TIRS images, with spatial resolution of 80 m and 30 m, respectively. ArcGIS 10.5 and ERDAS Imagine 14 are utilized for image processing. Maximum likelihood supervised classification method is performed to generate the signature class of significant land cover classes including agriculture, plantation/orchards, moderate forest, urban settlements, water bodies, woodland, dense forest, good rangeland, and moderate rangeland. For each classified images, an accuracy assessment step is executed using error matrix and Kappa coefficient followed by the post classification change detection analysis. To provide detailed information about the spatial and temporal variation of land use and land cover, the statics of changes in 1975 relative to 2015 were delineated using transition probability matrix. Our analysis suggests that around 351,000 hectares in Gilan province (equivalent to nearly 25% of land cover) has changed between 1975 and 2015. The results show that dense forest and plantation/orchards are disappearing with obtained change ratio of -5.76%, and -5.88%, respectively. Agriculture and urban settlements have been expanded about 91,900 ha and 29,000 ha, respectively. The majority of the converted land use types to urban settlements are identified as plantation/orchards, agriculture, and water bodies. Forest conversion to

other land uses, especially agriculture and plantation/orchards is highlighted in our analysis. The possible socio-economic impacts of these changes as well as their consequences on hydrologic processes in the region are discussed. Our investigation offers new insights regarding the changes in the land cover and land use in Gilan province of Iran which can guide future decisions, restorative land use practices, and contribute toward sustainable management of land, water and natural resources.

Keywords: Land use, Land cover, Sustainable management, Geographic information system, Remote sensing

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MS17 / 516

## Marangoni Effect Reshapes Drying Pattern in Porous Media

**Authors:** Yandong Zhang<sup>1</sup> ; Ke Xu<sup>1</sup>

<sup>1</sup> *Peking University*

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Drying or evaporation in porous media is always modeled as special scenario of classic fluid-fluid displacement. However, when the evaporation is extensive, the temperature at drying front can be much lower than other regions in the porous media and thus resulting in significant temperature gradient. Consequently, Marangoni effect may appear and reshape the fluid flow pattern, which has not been well investigated before. Such extensive drying in porous media normally occurs in CO<sub>2</sub> sequestration, gas condensate reservoir and shale gas recovery, fuel cell, water management, etc.

In this study, we conduct micromodel experiments to visualize the Marangoni effect during extensive drying in porous media. We fabricate a 2D transparent porous medium with an adjacent open fracture. The porous medium is saturated first with pentane, and air is then continuously injected to flow through the open fracture at different rates to control the pentane evaporation rates. Direct microscopic visualization is conducted to analyze the fluid flow pattern, and infrared camera is used to record the real-time temperature distribution.

We show that the drying pattern could be reshaped by the interplay between evaporation-induced Marangoni effect and viscous dissipation for liquid to supply the drying front. At high evaporation rate extreme, the main drying front stably moves inward to deep porous medium, as evaporation is much faster than liquid supply from deep; at low evaporation rate extreme, the main drying front moves in a classic capillary fingering pattern, as both the viscous dissipation and Marangoni effect are negligible. However, at intermediate evaporation rate, the air first invades deep into the porous medium through one single preferential path, and then scatters from the tip of this path to inner porous medium, while the main drying front keeps unmoved. In other words, the drying and displacement front are separated. Infrared camera records this phenomenon and support the above hypothesis of mechanism.

We further quantify the relationships of invaded pore sizes and distance from the initial invading front, with pore invasion trajectory, which illustrates the mechanisms laying under these three drying patterns. Dimensionless criterion that depicts the transitions among these regimes and therefore a phase diagram is yielded that matches experimental observation well. Further research will focus on how this Marangoni effect can impact Darcy-scale flow pattern.

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MS6-A / 393

## Material balance and mixing behavior during emulsification of crude oil by using micro-X-ray tomography

**Authors:** Mostafa Borji<sup>1</sup> ; Ahmad Kharrat<sup>None</sup> ; Rene Ritter<sup>2</sup> ; Pit Arnold<sup>None</sup> ; Holger Ott<sup>2</sup>

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The mixing behavior of oil and water is usually evaluated outside the pore space, under mixing conditions that does not correspond to porous media flow and by optical inspection. Especially the optical inspection disregards that, e.g., a little oil contamination in water may lead to a substantial coloring of the aqueous phase. A quantitative material balance is therefore difficult, if not impossible. In this study, we use the linear mass absorption coefficient of micro-X-ray tomography to establish the material balance during emulsification in classical test-tube experiments and in the porous medium under flow conditions.

With these methods we investigate the phase behavior and the displacement properties of crude oil from the Vienna Basin by alkaline injection waters with different Na<sub>2</sub>CO<sub>3</sub> concentrations. In alkaline flooding, in-situ surfactants are generated by saponification reactions between fatty acids and the alkali, which reduces the interfacial tension between oil and water and ultimately forms emulsion phases. In contrast to the ideal surfactant systems typically examined (surfactant solution and synthetic oil), emulsification leads to a more complex phase behavior that does not follow the classic Winsor regime and does not have clear optimal conditions.

We conduct and evaluate classic phase behavior experiments in test tubes, but by using micro-X-ray tomography. We show that the typical visual assessment is misleading and that for X-rays the assessment is conclusive and takes the material balance into account. We find the same fluid phase signature in micro-CT-based core flood experiments under flow conditions as in the test tubes. We show that, in contrast to earlier statements on the same system by other groups, a mutual minimal emulsification can be identified as optimal, which leads to the best recovery. Furthermore, micro-X-ray tomography provides spatial information about fluid distributions in the pore space and enables statements about the relative permeability and its changes.

The study shows the necessity of using X-ray-based methods to evaluate and quantify complex phase behavior as in case of complex crude oils and alkaline flooding. Using X-ray-based methods makes observations in test tubes and in the pore space comparable and leads to conclusive statements for injection water optimization.

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Poster + / 346

## Mathematical Modeling of the Effect of Acoustic Waves on oil Recovery in Porous Media

**Authors:** Harris Rabbani<sup>1</sup> ; Albertus Retnanto<sup>None</sup> ; Mahmood Amani<sup>None</sup>

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To this day, the petroleum industry is still searching for alternative ways to improve hydrocarbon recovery from the reservoir. The residual oil blotches may consist of about 30% - 40% or more of a volume fraction. The interest in applying Enhanced Oil Recovery (EOR) techniques on the additional amount of oil is because conventional methods cannot produce it. EOR is one option of the technologies required to increase reserves. EOR technologies such as chemical injection, gas injection, or thermal processes are not applicable for all reservoir conditions. Issues such as injectivity stability, oil composition, mineral precipitation, and reservoir depth serve as a first estimation of when a method should be implemented in a given reservoir. The increase in oil production due to seismic activity has been reported for more than 70 years and can be considered an effective EOR technique. In this research, we present a novel analytical framework that can forecast the oil recovery as a result of acoustic vibrations. The presented analytical model aids in improving understanding of various properties influencing oil recovery as a result of acoustic vibrations. Our analytical model is validated against series of experimental data under different boundary conditions. The proposed model may be further integrated into the reservoir simulation to improve their predictive capabilities.

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MS17 / 226

## Measuring The Anisotropic Heat Transfer Coefficients In Carbon Fiber Felt

**Author:** Shaolin LIU<sup>None</sup>

**Co-authors:** Azita Ahmadi ; Hermes Scandelli ; Cyril Levet ; Jean Lachaud

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Thermal protection systems (TPS) are used to ensure acceptable temperatures for the outer surface of a spacecraft during all mission phases and particularly during atmospheric re-entry. Carbon fiber felt is widely used in TPS systems due to its high porosity and low thermal conductivity [1]. It is an anisotropic material. In local thermal non-equilibrium (LTNE) models, a heat transfer coefficient (HTC) is used to represent the internal heat exchange between the fluid and solid phases. Some correlations for metal foams, packed beds and ceramic foam are proposed in the literature for the prediction of the HTC [2]. However these correlations are not suitable for carbon fiber felt due to its geometric parameters, namely smaller fiber diameter (50 $\mu$ m), lower thermal conductivity (0.23W/(m<sup>3</sup> K)) and its anisotropic structure. In this work, an inverse method was used to determine the anisotropic HTC between a gas stream and a carbon fiber felt sample. This method consists of three steps: transient single-blow technique (TSBT) experiments, macroscopic numerical simulation and error minimization between the results of the two first steps. To investigate the influence of the anisotropic structure of the materials on HTC, different experiments were performed by changing the orientation of the sample (Through-Thickness (TT), In-Plane (IP)), the inlet gas velocity varying from 0.23m/s to 0.94m/s. The experimental data are input into the macroscopic simulation process as initial and boundary conditions. The computational area includes a fluid (gas flow in the tube) and a porous domain. The energy conservation equations are solved using a finite volume method in the Porous material Analysis Toolbox based on OpenFoam (PATO) [3]. Besides, a numerical model of the

thermocouple allowed to compute the temperature difference between the gas and the thermocouple probe. At last, a method for minimizing the error between calculated and measured temperatures is introduced, so that we can get the most suitable value of HTC. When the orientation of the sample is changed while keeping the same conditions, different values of the HTC are found. To take explicitly into account the flow direction, a new formulation with HTC has been proposed. This formulation will also be verified using pore-scale simulation in the future [4].

Keywords: Local thermal non-equilibrium; Anisotropic materials; Macroscopic numerical simulations; error minimization

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MS6-A / 102

## Measuring and modelling multi-scale fluid distributions in heterogeneous rocks based on X-ray micro-computed tomography

**Authors:** Shan Wang<sup>1</sup>; Leo Ruspini<sup>2</sup>; Stefanie Van Offenwert<sup>1</sup>; Arjen Mascini<sup>3</sup>; Tom Bultreys<sup>1</sup>

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Multiphase flow through heterogeneous reservoir rocks is commonly found in geoscience applications. The accurate characterization of the pore space topology and fluid flow mechanisms is crucial to predict reservoir performance. This can be studied by visualizing the pore space with micro-computed tomography, allowing to construct image-based models (Bultreys et al., 2016). However, the multi-scale nature of many reservoir rocks typically results in significant amounts of sub-resolution porosity in micro-computed tomography (micro-CT) experiments. The challenging nature of multiphase flow simulations in such pore geometries has spurred the development of multi-scale models, such as dual pore network models (Jiang et al., 2013; Bultreys et al., 2015) and Stokes-Brinkman solvers (Menke et al., 2019). However, these models depend strongly on input parameters and physical assumptions describing the microporosity. There is currently a lack of direct validation methods to reduce the associated uncertainties in such simulations.

In this presentation, we present a pore-scale validation workflow based on an unsteady-state drainage experiment on an Estailades limestone sample, imaged with micro-CT. Contrast agent-based difference imaging (Ghous et al., 2014; Boone et al., 2014; Lin et al., 2017) was used to first generate a sub-resolution porosity map of the sample and to then map the sub-resolution fluid saturations at several capillary pressure steps during the drainage. To this end, the sample was first saturated with high concentration KI-doped brine solution (25 wt%), and then displaced by n-decane with gradually increased drainage pressure (8 kPa-400 kPa). The resulting experimental data shows a good agreement with the mercury intrusion capillary pressure (MICP) curve for Estailades (Bultreys et

al., 2015). Then, the sub-resolution porosity map was used to generate a multi-scale pore network model of the sample studied in the experiment. Drainage simulations on this network model were validated by comparison to the experimental saturation maps on a pore-by-pore basis. The method can be used to inform and validate multiphase flow simulation in complex rock types, which is crucial to extend the use of digital rock physics for complex reservoir rocks.

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## Measuring co-diffusion kinetics on thin films

**Author:** Meishan Guo<sup>1</sup>

**Co-author:** Majid Naderi<sup>1</sup>

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Moisture transport characteristics of porous materials play an important role in many industries. For example; packaging materials which can be directly related to shelf life and packaged product stability; model membranes which are widely used in in-vitro permeation studies in skin care industry; and electrospun nanofibres for polymeric scaffolds. Moisture vapour transmission rate (MVTR) measurements are generally carried out under isothermal conditions and describe the rate of water permeating through a test specimen into the headspace volume of a container which differs in relative humidity ( $\Delta RH$ ).

Dynamic gravimetric vapour sorption (DVS) is a well-established method for the determination of vapour sorption isotherms. The high mass resolution and excellent baseline stability of DVS allows the fast and accurate determination of water sorption isotherms and diffusion kinetics over a wide range of temperature and humidity. DVS equipped with Speed of Sound sensor, is a very sensitive tool to measure organic vapour sorption and desorption. Furthermore, it is also capable of studying co-adsorption isotherms using two vapours, or organic vapour sorption at a particular relative humidity background. DVS instrument therefore can be used to determine co-diffusion kinetics on thin film samples. In this study, the diffusion of methanol, water and water-methanol co-diffusion through Kapton film at different temperatures were investigated using a specially designed Payne diffusion cell and DVS instrument.

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1: Surface Measurement Systems Ltd., Unit 5, Wharfside, Rosemont Roan, Alperton, London, HA0 4PE, UK

2: Surface Measurement Systems Ltd., 2125 28th street SW, Suite 1, Allentown, PA 18103, USA **Acceptance of Terms and Conditions:**

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**MS13 / 481**



## Mechanisms of gas separation through 2D porous graphene membranes : theory and molecular simulations

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In a context of energy transition, the growing share of gas (natural gas, hydrogen, bio-gas) in the energy mix, as well as the need to store CO<sub>2</sub> and reduce its emissions, calls for an improvement in gas separation techniques. In this sense, free standing nanoporous graphene is a promising material because it makes it possible to exceed the selectivity to permeance ratio of other membrane materials.

In this study, we use molecular simulations to document the physical mechanisms governing permeation and gas separation through 2D graphene membranes, for different pore sizes and a range of thermodynamic conditions. Our objective is to identify, understand and quantitatively predict the transport properties of gases through these materials.

For pure species, we show that the permeation of a gas molecule consists of two successive steps: the permeation of the membrane plane through the pore and the desorption from the graphene sheet to the bulk. The first step is driven by steric effects in the pore plane. The second stage is the result of a competition between desorption kinetics and surface diffusion along the graphene sheet since an adsorbed molecule can recross the pore or diffuse towards another as long as it does not desorb. On the basis of these observations, we propose a theoretical model that allows us to reproduce the results of the simulations. This model shows that the potential of mean force between a permeating gas molecule and the graphene atoms in the pore region plays a central role.

In addition, we have simulated the separation of gas mixtures (CH<sub>4</sub> / CO<sub>2</sub>, O<sub>2</sub> / N<sub>2</sub>) through various nanoporous graphenes to investigate the selectivity of this type of membrane. Our data show the limits within which the results obtained for pure gases can be used to predict the separation of mixtures.

We believe that these recent results are of interest to help optimise the design of 2D graphene-based membranes, both from the point of view of the geometry or spatial distribution of the pores and their chemical functionalization.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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Poster + / 196

## Meshless Lattice Boltzmann Method for pore-scale porous media flow

**Authors:** Dawid Strzelczyk<sup>None</sup> ; Maciej Matyka<sup>1</sup>

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We will present our recent results on the development of semi-Lagrangian meshless Lattice Boltzmann method and its application to porous media flows. Our approach for meshless LBM will be similar to 1. Here however we will operate on non-regular discretizations. Thus, it will be possible to easily refine discretization e.g. in narrow passages of pore-space. Results on velocity fields and results analysis will be presented.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

1 Lin, X., Wu, J., & Zhang, T. (2019). A mesh-free radial basis function-based semi-Lagrangian lattice Boltzmann method for incompressible flows. *International Journal for Numerical Methods in Fluids*, 91(4), 198–211. <https://doi.org/10.1002/flid.4749> **Acceptance of Terms and Conditions:**

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MS4 / 169

## Mesoporous, Moisture-Absorbent, Temperature-Controlled Hydrogels For Atmospheric Water Harvesting

**Authors:** Galen Mandes<sup>1</sup> ; Sujit Datta<sup>2</sup> ; Jean-Francois Louf<sup>1</sup> ; Xiaohui Xu<sup>1</sup> ; Rodney Priestley<sup>1</sup> ; Sankaran Sundaresan<sup>1</sup>

<sup>1</sup> *Princeton University*

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Water scarcity is one of the biggest challenges of the 21st century. Using desiccants to harvest water from air is a promising way to address this challenge. However, most desiccants require considerable energy input to release absorbed water as vapor and then condense it. Here, we overcome this limitation by developing Moisture-Absorbent, Temperature-Controlled Hydrogels (MATCHes) that absorb water from air at ambient conditions, and then release it in liquid form upon slight heating. Furthermore, we show that tuning the mesoscale porosity of the hydrogels dramatically impacts both the total amount and rate of water absorption and release – highlighting a previously-overlooked factor that regulates MATCH performance. Our work therefore demonstrates a new route to fabricating desiccants capable of harvesting water from air quickly, to a large extent, and with minimal energy cost.

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MS17 / 16

## Mesoscale Modelling of Thermal-Chemical processes during Nuclear Fuel Corrosion

**Author:** Min Liu<sup>None</sup>

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Understanding corrosion mechanisms and processes of UO<sub>2</sub> fuel is essential for safe operation of nuclear reactors and storage of spent fuel [1-3]. We develop a 3D physics-based numerical model to simulate the thermal-chemical process during the corrosion of UO<sub>2</sub> fuel pellets. Mass transfer, thermal conduction and solid chemical reactions are coupled in the model. The impact of temperature on uranium speciation during fuel corrosion is investigated. The UO<sub>2</sub> pellets lifetime under corrosion is compared at same temperature but different reactions. The predicted reaction rates are shown to be dependent on the reaction types. The impact of microfractures on fuel pellets corrosion are studied by modelling reactions in fractured pellets. The composition change caused by radiation is also explored. The fuel with UO<sub>2</sub>-U<sub>3</sub>O<sub>8</sub> mixture is constructed. The results show the mixed fuel presents faster reaction rates in comparison with pure UO<sub>2</sub> samples. The developed model will help quantify the effect of temperature on nuclear fuel dissolution and, help determine the key parameters controlling the physiochemical processes and ultimately inform the nuclear industry.

### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

- [1] Liu, M., Kang, Q., & Xu, H. Grain-scale study of the grain boundary effect on UO<sub>2</sub> fuel oxidation and fission gas release under reactor conditions. *Chemical Engineering Science*, 229, 116026.  
[2] Liu, M., Kang, Q., & Xu, H. (2020). Modelling uranium dioxide corrosion under repository conditions: A pore-scale study of the chemical and thermal processes. *Corrosion Science*, 108530.  
[3] Liu, M., & Mostaghimi, P. (2018). Reactive transport modelling in dual porosity media. *Chemical Engineering Science*, 190, 436-442. **Acceptance of Terms and Conditions:**

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MS19 / 185

## Mesoscopic modeling of porous media with application to electrochemical energy conversion and storage devices: the case of gas diffusion layers and proton-exchange membranes

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Porous media are an integral part of energy conversion and storage electrochemical devices. Among them, we have gas diffusion layers (GDLs) and catalyst layers used in polymer electrolyte membrane fuel cells (PEMFCs), as well as fibrous electrodes used in redox flow batteries (RFBs) [1-10]. These porous media must fulfill several critical functions, such as providing a transport pathway for reactants/products through its pore volume and ensuring charge and heat conduction through its solid structure. Catalyst layers and active electrodes have the added functionality of providing a reactive surface area. Conduction in proton-exchange membranes (PEM) through water-filled ionic channels can also be modeled using percolation theory [11].

In this talk, an overview of mesoscopic modeling approaches applied to transport in GDLs and PEMs is presented. A composite continuum-pore network formulation is used to model two-phase transport in GDLs [9,10]. The composite model incorporates a control volume mesh at the layer scale, which embeds a structured cubic pore network. Capillary transport is simulated using the discrete pore network, considering the Purcell toroid model to determine the local entry capillary pressures of the fibrous material. The pore-network model is also used to determine analytically local anisotropic effective transport properties (local effective diffusivity and permeability), which are mapped onto

the CV mesh to simulate transport within the porous layer using a continuum formulation. As a second example, proton conduction in multiblock copolymer membranes is modeled based on percolation theory [11]. The mesoscopic model solves simplified Nernst-Planck and charge conservation equations on a random cubic network. To mimic experimental conditions, hydrated sulfonated sites not connected to the edges of the domain are excluded from the network.

A comparison with experimental data is presented in terms of capillary pressure curves, water distribution and effective diffusivity in carbon-paper GDLs, as well as proton conductivity and water uptake in multiblock copolymer membranes of sulfonated polysulfone and polyphenylsulfone.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

- 1 P.A. García-Salaberri et al., *J. Power Sources* 359 (2017) 634–655.
- [2] P.A. García-Salaberri et al., *Processes* 8 (2020) 775.
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- [7] Z.A. Khan, P.A. García-Salaberri, T. Heenan, R. Jarvis, P. Shearing, D. Brett, A. Elkamel, J.T. Gostick, *J. Electrochem. Soc.* 167 (2020) 040528.
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- [9] P.A. García-Salaberri et al., *ECS Trans.* 97 (7) 615.
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**Poster + / 314**

## Methane adsorption on Silica-Kaolinite interface for shale gas application: A theoretical study

**Author:** Abdulmujeeb Onawole<sup>1</sup>

**Co-authors:** Mustafa Nasser<sup>1</sup>; Ibnelwaleed Hussein<sup>1</sup>; Mohammed Al-Marri<sup>1</sup>; Ahmad Sakhaee-Pour<sup>2</sup>; Santiago Aparicio<sup>3</sup>

<sup>1</sup> *Qatar University*

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Methane mostly makes up the constituent of shale gas and it is currently being exploited in fulfilling the world's energy demands 1. Molecular simulation techniques including Density Functional Theory (DFT) and Molecular Dynamics (MD) techniques are employed to understand methane transport in the pores at typical reservoir conditions [2]. To simulate the shale model which in reality is made up of clay and quartz-like material, an interface is created from the pure surfaces of silica (quartz) and kaolinite (clay) [3,4]. The simulations revealed that the interface is formed by a chemical bond between a silicon atom from the silica surface and two oxygen atoms from the kaolinite surface. The adsorption of methane was studied at three different positions on the Silica-Kaolinite interface namely, silica-dominated region, interface region, and kaolinite-dominated region. The mode of adsorption of methane irrespective of its position on the interface was found to be physisorption [5]. However, methane has stronger adsorption on the kaolinite region than the silica region. This

results provides insight at the molecular level of methane interaction with a silica-kaolinite interface which will be useful in shale reservoir application particularly in estimating the original gas in place.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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## Method for predicting a reasonable water injection pressure for a fractured low-permeability sandstone reservoir

**Author:** Jingshou Liu<sup>1</sup>

<sup>1</sup> *China University of Petroleum, East China*

**Corresponding Author:** liujingshou@126.com

In the process of fractured reservoir development, fracture opening pressure, opening sequence, and reservoir fracture pressure are the factors that must be considered when formulating oil and gas development plans. Particularly in fracturing, refracturing, and water injection development measures for a low-permeability reservoir, accurate prediction of structural fracture development law and reservoir fracture pressure is an important guarantee of improved oil and gas recovery and economic benefits. A reasonable injection pressure for oil and gas wells cannot exceed the fracture pressure of oil and gas reservoirs. Under this pressure condition, the structural fractures should be fully opened to maximize the oil and gas recovery efficiency. Through structural evolution analysis, combined with rock fracture criteria, the occurrence of fractures is predicted; based on the theory of fracture surface energy and rock strain energy in fracture mechanics, the linear fracture density is predicted. Using a core sound velocity experiment and microseismic monitoring technology, the in situ stress direction is determined. Combined with the fracturing data, the in situ stress of each well is calculated; by determining the rock mechanics parameters and a finite element model, the three-dimensional distribution of the in situ stress can be predicted; with the aid of the fracture occurrence and the stress field numerical simulation results, the reservoir fracture pressure and the opening sequence of natural fractures in the reservoir are determined. We used the Paleogene Funing Formation in the T96 fault block of the Jinhua Sag in eastern China as an example to predict the reasonable water injection pressure of fractured low-permeability reservoirs. Observations of core fractures in the Funing Formation in the T96 fault block show that the predominant orientation of fracture strikes is ENE and WNW conjugate fractures; the dip consists of mainly vertical fractures and high-angle oblique fractures (87%). The simulation results of the stress field show that the horizontal minimum principal stress is between 21 MPa and 28 MPa, and the maximum horizontal principal stress is between 30 MPa and 40 MPa. The horizontal maximum principal stress of the T96 fault block is in the ENE direction; near the fault, the direction of the horizontal principal stress changes by 5° to 10°. During water injection, the fractures in the ENE direction open first, and the

fractures in the SE direction open subsequently. The opening pressure of the fracture increases as the angle between the fracture strike and the horizontal maximum principal stress becomes larger; the depth of the fracture and the opening pressure are also positively well correlated. In the high part of the structure (1650 m-2000 m), the fracture opening pressure is between 22 MPa and 42 MPa at the opening and between 41 MPa and 69 MPa in the lower portion of the structure (3150 m-3800 m). By calculating the actual fracture pressure of the reservoir, it is proposed to use different water injection pressures in different blocks to ensure high and stable oil and gas well production.

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MS24 / 276

## Micro-macro Modeling Approaches for Reactive Multiphase Flow and Transport in Complex Media

**Authors:** Peter Knabner<sup>1</sup> ; Nadja Ray<sup>2</sup> ; Stephan Gärttner<sup>3</sup>

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<sup>2</sup> Friedrich-Alexander Universität Erlangen-Nürnberg

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In porous media and other complex media with different length scales, (periodic) homogenization has been successfully applied for several decades to arrive at macroscopic, upscaled models, which only keep the microscopic information by means of a decoupled computation of 'effective' parameters on a reference cell. The derivation of Darcy's law for flow in porous media is a prominent example. Numerical methods for this kind of macroscopic models have been intensively discussed and in general are considered to be favourable compared to a direct microscale computation. On the other hand, if the interplay of processes becomes too complex, e.g. the scale separation does not act in a proper way, the porous medium itself is evolving, ..., the upscaled models obtained may be *micro-macro models* in the sense, that the coupling of the macroscopic equations and the equations at the reference cell is both ways, i.e. at each macroscopic point a reference cell is attached and the solution in the reference cell depends on the macroscopic solution (at that point) and the macroscopic solution depends on the microscopic solutions in the reference cells. At the first glance such models seem to be numerically infeasible due to their enormous complexity (in  $d + d$  spatial variables). If on the other hand this barrier can be overcome, micro-macro models are no longer a burden but a chance by allowing more general interaction of processes (evolving porous media, multiphase flow, general chemical reactions, ...), where the microscopic processes 'compute' the constitutive laws, which need longer be assumed (similar to the concept of heterogeneous homogenization). We will discuss various examples and in particular numerical approaches to keep the numerical complexity in the range of pure macroscopic models.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

S. Molins and P. Knabner, Multiscale Approaches in Reactive Transport Modeling, Reviews in Mineralogy & Geochemistry, 85.1, pp. 27–48, 2019.

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Efficiency and Accuracy of Micro-Macro Models for Mineral Dissolution, Water Resources Research 56, e2020WR027585, 2020. **Acceptance of Terms and Conditions:**

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MS1 / 552

## Micro-scale Insights into the Effects of Ionic Strength on CO<sub>2</sub> Induced Carbonate Rocks Dissolution

**Authors:** Shima Ghanaatian<sup>1</sup> ; Omid Shahrokhi<sup>1</sup> ; Susana Garcia<sup>1</sup> ; Mercedes Maroto-Valer<sup>1</sup>

<sup>1</sup> Heriot-Watt University

**Corresponding Authors:** s.garcia@hw.ac.uk, o.shahrokhi@hw.ac.uk, m.maroto-valer@hw.ac.uk, sg116@hw.ac.uk

Deep saline aquifers are appropriate for the long-term storage of captured CO<sub>2</sub>. Low pH environments of deep aquifers due to CO<sub>2</sub> injection and dissolution would trigger rock dissolution while the extent of rock dissolution depends on the brine chemistry[2]. Carbonates are the main mineral forming the matrix of carbonate rocks[3]. Moreover, carbonate minerals show higher kinetic reactivity in comparison with aluminosilicate minerals, and therefore, these are the first minerals that react with acidic fluids. Our previous study showed that the brine chemistry affects the extent of carbonate mineral dissolution and consequently, the micro-scale structure and porosity ( $\Phi$ ) of the reservoir rock[2].

Even though it is well known that the aqueous phase in geological reservoirs has ionic strengths ranging up to several hundred g/L, the role of this parameter on geochemical rock-fluid interactions is still a subject of debate in the literature[2][4] due to the variety and complexity of the employed rock and fluid compositions. Thus, this research aims to ascertain the relationship between the alteration of micro-scale pore structure of Indiana limestone, as a common carbonate reservoir rock (>98% calcite) and change in ionic strength of reactive CO<sub>2</sub>-saturated brine. Three static experiments were designed to evaluate the effect of ionic strength on the amount of CO<sub>2</sub>-saturated brine induced rock dissolution, using various analytical methods. Brines were synthesized by the most common types of ions[5] which are found in deep aquifers including Na<sup>+</sup>, K<sup>+</sup>, Mg<sup>2+</sup>, Ca<sup>2+</sup>, and Cl<sup>-</sup>, to reach ionic strengths from 0 to 0.6 mol/L. Indiana core plugs (with dimensions of 5mm×12mm in diameter and length, respectively) were initially equilibrated with brines for 25 days, based on the geochemical modeling. Then CO<sub>2</sub> was injected into hydrothermal batch vessels at a pressure of 130 bar and temperature of 60°C that are representative of subsurface reservoir conditions. Experiments with CO<sub>2</sub> saturated brines were continued for 14 days to ensure that desired rock-fluid interactions have occurred. Brine samples (2 mL) were collected at each step to analyze the Ca<sup>2+</sup> concentration using inductively coupled plasma-optical emission spectroscopy (ICP-OES) technique.

A Micro-computed tomography ( $\mu$ -CT) scanner was used as a non-invasive methodology for obtaining information on the spatially resolved three-dimensional pore structure of the rock. Images were acquired with a 4  $\mu$ m spatial resolution and X-ray beam of 80 keV and 80 $\mu$ A before and after each experiment to evaluate the changes induced by CO<sub>2</sub>-saturated brine. The alterations of macro-porosity, interparticle sub-resolution micro-porosity, and solid phase of the rock were assessed by  $\mu$ -CT images. The results of the ICP-OES were used to compare the amount of released Ca<sup>2+</sup> in the brine with the calculated volume of dissolved rock by  $\mu$ -CT images. Overall, results of ICP-OES and  $\mu$ -CT images illustrate that the extent of rock dissolution and alteration of pore structure of rocks were depending on the ionic strength of the solutions. Therefore, higher ionic strength leads to more rock dissolution. Good agreement was also observed between the total porosity calculated from  $\mu$ -CT images ( $\Phi = 0.203$ ) and helium porosity measurements ( $\Phi = 0.215$ ).

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1 Y.-M. Wei et al., "A proposed global layout of carbon capture and storage in line with a 2° C climate target," *Nat. Clim. Chang.*, pp. 1–7.

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MS5 / 420

## Microbial Induced Desaturation and Precipitation (MIDP) in Stratified Granular Soil

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A meter-scale tank test simulating two-dimensional plane strain conditions was performed to evaluate the effectiveness of microbially induced desaturation & precipitation (MIDP) through denitrification for ground improvement applications in stratified soils. The process stimulates indigenous nitrate-reducing bacteria through the injection of a solution containing nitrate, calcium and a dissolved organic carbon source and results in the production of biogenic gas, biominerals and biomass. Entrapped gas bubbles can dampen pore pressures under cyclic loading, while biominerals form cementing bridges between existing grains, making MIDP a viable ground improvement technique for liquefaction hazards in granular soils. Desaturation of the soil requires a much lower amount of treatment than precipitation, however, precipitation may provide a more durable stabilizing effect as the entrapped gas may migrate and vent to the atmosphere. Previous studies have demonstrated the mechanical response for treated granular soils at bench scale, however limited knowledge is available on the impact of partial desaturation on the hydraulic properties of the soil, particularly in stratified formations. Further investigation into this area is important for the up-scaling and future commercialization of the process as it may affect injection strategies, and the distribution of substrates and metabolic products. The process was monitored in terms of changes in electrical conductivity, moisture content, pore pressure and flow velocity. The results demonstrate how stratification affects the process performance and identify the challenges associated with treatment of layered soil systems.

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MS11 / 412

## Microfluidic and numerical investigation of recirculation induced reaction hot spots in a porous media analog

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**Corresponding Authors:** pkkang@umn.com, chen7007@umn.edu, lee02258@umn.edu

While flow in porous media systems, such as in groundwater and rock fracture flow, is usually laminar ( $Re < 500$ ), it has been increasingly recognized that recirculating flow structures can appear in these systems even at  $Re$  numbers less than one [1,2]. Furthermore, the structure of porous media leads to fluid stretching and folding that dramatically alters the fate of solutes, even in the absence



of inertial forces and recirculating (vortical) flows [3]. These conditions should operate in tandem to significantly impact mixing and reaction in porous media, processes that are central to the fate of groundwater contaminants and biogeochemical cycling of nutrients. Previous work with a chemiluminescent reaction at a straight channel cross intersection showed that 3D vortical flow structures form and create reaction hot spots for  $Re$  numbers as low as 100 [4]. Another study showed that vortical flow structures can control transport processes even in low  $Re$  number ( $Re \ll 1$ ) porous media flow, but further work is needed to examine how recirculating flows influence mixing and reaction in porous systems [5]. The overarching goal of this work is to identify the physical (pore structure), hydrodynamic ( $Re$ ), and chemical (reaction rate) conditions where recirculating flows create reaction hot spots in a porous media.

Here, we combine 3D pore-scale numerical simulations and microfluidic experiments with a bimolecular chemiluminescent reaction to study the formation of recirculation induced reaction hotspots in low to moderate  $Re$  number flows. We use a microfluidic channel as a porous media analog where two reactants are injected into separate channels that converge to a central channel containing a sequence of pillars that represent grains of a porous media. By adjusting the flow condition ( $Re$ ) and spacing of the pillars, recirculation can be readily induced within the space between the pillars. The appearance of the reaction hot spots then depends on the interplay between the factors creating recirculating flow, and the kinetics of the chemical reaction. The results of this work show that the critical  $Re$  to initiate recirculation is sensitive to pore geometries and well within the range of flow conditions common to natural soils and fractures. We also demonstrate that even once recirculation has formed, there is an optimal flow condition which enhances the reaction rate, which is controlled by the balance of flow velocity against reaction time scale. These results imply that typical soil porous media geometries, hydrodynamic conditions, and geochemical reactions will readily create vortical structures that induce reaction hot spots which will play a significant role in many natural porous media and fractured systems. During mineral precipitation and dissolution for example, recirculation induced reaction hot spots may drive preferential reaction in certain locations, which will influence evolution of porosity as the reactions proceed.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

- 1 D. L. Koch and R. J. Hill, Inertial Effects in Suspension and Porous-Media Flows, *Annu. Rev. Fluid Mech.* 33, 619 (2001).
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MS6-B / 782

## Microfluidic investigation of phase banking during low tension displacements

**Author:** Lucas Mejia<sup>None</sup>

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During low tension displacements, aqueous surfactants are injected into porous rocks to mobilize trapped oil or non-aqueous phase liquids (NAPLs). The trapped ganglia move and form aggregations (banks) that are a considerable fraction of the flow domain (~0.1 to 0.5 domain length). Formation of phase banks during low tension displacements has been widely observed in corefloods in the context of enhanced oil recovery and NAPL remediation. Additionally, fractional flow theory provides a macro-scale explanation for the formation of banks: if the velocity of the saturation of the oil bank is larger than that of the injectant, a bank should form. However, the pore-scale mechanics of banking are not clear and have not been widely investigated, likely because banking appears to be scale dependent and most direct-imaging platforms capture small flow domains. Why do oil ganglia coalesce and move as a bank, rather than as individual ganglia? How are the surfactants distributed within and around the bank? Using a novel microfluidic platform, a “coreflood on a chip”, we visualize aqueous surfactant solution displacing oil at varying viscosity ratios and try to answer these questions. We find that banks may form at very unfavorable viscosity ratios, and the presence of surfactant in a region at the rear of the bank is necessary for the oil bank to form.

The coreflood-on-a-chip is a glass micromodel that is 1.2ft long, has a heterogeneous pore structure, and includes shallow, 2.5D pore throats (Mejia et al., 2020). Our experiments involved injecting brine (30,000 ppm Na<sub>2</sub>CO<sub>3</sub>, 1 cp) into the micromodel, displacing the brine with a viscous crude oil from the Alaskan North Slope (0.81 g/cm<sup>3</sup>, 83 cp), displacing the crude oil with 30,000 ppm Na<sub>2</sub>CO<sub>3</sub> until residual oil saturation was reached, and finally injecting aqueous surfactant solution (mixture of a sulfate anionic surfactant, an internal olefine sulfonate, and IBA) continuously. We adjusted the viscosity of the surfactant solution by including hydrolyzed polyacrylamide (HPAM) to achieve viscosities of 1 cp (without polymer), 40 cp (with 2400 ppm polymer), and 90 cp (with 3600 ppm polymer). The water-oil displacements were conducted at 8 ft/day, while the surfactant solution-oil displacements were conducted at 4 ft/day. Whole domain images were captured using a digital single lens reflex camera, and pore-scale images were captured using a stereomicroscope. Results from the whole domain images were interpreted using fractional flow theory, and discrepancies between experimental results and the model are explained using the microscopic images. Furthermore, we conduct pore-scale simulations using the Volume of Fluids (VOF) method in a simple geometry to interpret the experimental results recorded using the stereomicroscope.

Our experiments show some surfactant must be present at the rear of the oil bank to initiate its formation. Moreover, the distribution of surfactant solution is more nuanced than that described by fractional flow; some surfactant is present within the oil bank. Finally, the pore-scale simulations indicate radial dispersion of oil and interfacial tension gradients (at the pore-scale) are important mechanisms for bank formation.

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## **Microscale modeling of thermo-hydro-mechanical behavior of fruit tissue during drying**

**Author:** Xinzhu Mou<sup>1</sup>

**Co-author:** Zhenqian Chen <sup>1</sup>

<sup>1</sup> *Southeast University*

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The deformation of fruit tissue caused by drying typically results in consequent quality loss. To better understand the mechanism of heat and moisture transfer, a coupled thermo-hydro-mechanical model was developed at microscopic cell scale. Pear was chosen as the research object as this fruit suffers from great shrinkage after drying. A 2D geometric model of cortex tissue was obtained by a virtual fruit tissue generator that is based on cell growth modeling. The distribution of temperature and moisture in tissue cells were predicted using transport laws, and the different physical

properties of the microstructural components were obtained experimentally or from literature. An equivalent microscale cell model that incorporates the dynamics of mechanical deformation of the cellular structure was implemented. It can not only predict the heat and moisture transport in tissue cells, but also obtain the deformation characteristics of different regions in the tissue, which further reveals the thermo-hydro-mechanical coupling mechanism during drying process. The results showed that the pore size of tissue cells gradually decreased with time. At a drying temperature of 70°C, the volume shrinkage ratio of tissue cells was about 50% after reaching a steady state. The intercellular spaces of tissue can be regarded as closed pores in porous media, and stress concentration tends to occur near these positions. A sensitivity analysis of water permeability, thermal conductivity of cell membrane and elastic modulus of cell wall on the tissue deformation showed that, the cell membrane permeability has a greater impact on the deformation during drying within a certain range of changes. It will then become feasible to evaluate measures to improve the quality of fruits and vegetables during drying using this model in a multiscale modeling framework.

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MS20 / 316

## Microstrokes and capillary dilations – investigating the effect of single capillary alterations

**Authors:** Franca Schmid<sup>1</sup> ; Giulia Conti<sup>None</sup> ; Bruno Weber<sup>2</sup> ; Patrick Jenny<sup>None</sup>

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Capillaries are the most frequent vessel type of the brain's vasculature. The dense and highly interconnected capillary bed is key to ensure a robust blood supply over the entire depth of the cortex, and during baseline and neuronal activation. Besides its relevance our knowledge of structural and functional properties of the capillary bed remains limited. We perform blood flow simulations in realistic microvascular networks and alter individual capillaries to improve our understanding of capillary perfusion and robustness. More precisely, we first investigate the impact of single capillary dilation (1), which has been suggested as a mechanism to contribute to up-regulate flow during neuronal activation. Subsequently, we study flow changes in response to single capillary occlusion (2), because these micro-lesions are linked to dementia and Alzheimer's disease. Both studies provide insights on the role of these alterations but importantly also regarding general characteristics of the cortical capillary bed. Additionally, thanks to our numerical model which tracks 100 thousands of red blood cells (RBCs) (3), we are able to comment on the impact of RBCs on these local changes.

Our results show that a capillary dilation of 10% leads to a flow increase of 23% (per 100  $\mu\text{m}$ ) and an increase in the number of RBCs of 20% in the dilated capillary. Interestingly, the precise response depends on the relative bulk flow velocity difference at the upstream divergent bifurcation. As such, single capillary dilation causes a local increase in flow rate and a redistribution of RBCs. However, to increase the total inflow by ~6% in a microvascular network embedded in a tissue volume of 1 mm<sup>3</sup> all capillaries need to dilate by 10%. Consequently, capillary dilation is likely relevant for a localized redistribution of flow and RBCs, but is not the driving force to induce an overall flow increase.

Comparable to single capillary dilations, the effects of a microstroke are most pronounced in the direct vicinity of the microstroke capillary (MSC) and the severity is governed by the local vascular

topology. The largest changes are observed for a MSC with a convergent bifurcation upstream and a divergent downstream (2-in-2-out). Here, the flow rate drops by 80% in the directly adjacent vessels and is still reduced by 20% in generation  $\pm 3$  from the MSC. Significantly, smaller changes are observed for a MSC with a divergent bifurcation upstream and a convergent bifurcation downstream (1-in-1-out). Interestingly, MSCs of type 2-in-2-out are considerably less frequent than MSCs of type 1-in-1-out. Moreover, they supply a significantly smaller tissue volume with oxygen and nutrients. Taken together, our results suggest that the perfusion of the capillary bed is inherently robust to single capillary occlusions. Moreover, we hypothesize that the different topological configurations might fulfil distinct structural and functional tasks.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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## **Microstructural Evolution of Sand Assembly in Direct Shear Test: An Experimental Study using X-Ray Tomography**

**Authors:** Lalit Kandpal<sup>1</sup> ; Anurag Gautam<sup>2</sup>

**Co-authors:** Nimisha Roy<sup>3</sup> ; Satoshi Matsumura<sup>4</sup> ; Prashanth Vangla<sup>5</sup> ; J. David Frost<sup>3</sup>

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<sup>2</sup> *Department of Civil Engineering, Indian Institute of Technology Dehli*

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The macroscopic mechanical behaviour of granular-porous media is largely influenced by kinematics of its micro-mechanical counterparts of particles and pores. Deformation at particle-level is not uniform across a granular sample but is localized along the directional force chain, thus forming shear intensive failure surface known as shear zone. This results in complex internal failure mode and therefore, judgements from surface deformations using digital imaging techniques may be misleading. With the aid of 3D imaging techniques, microscopic variation at the particulate level can be studied. This study presents the localized evolution of the microstructural particle and pore properties in sand assemblies with different particle sizes. Direct shear test is conducted on two sand specimens with different particle sizes inside an x-ray scanning environment. The scanned images at various stages of the tests are pre-processed using algorithms implemented in MATLAB. The micro-scale properties of particle and pore data are extracted from each scanned image. For analysing the localized evolution of microstructure during shearing, the stacked data of both specimens are studied using SPAM [2]. The influence of particle size on the evolution of microstructural particle and pore properties and consequently on macroscopic response of the specimen is investigated in detail.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

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## Microstructure changes of oilwell cement enhanced by micro crystallized Ca-montmorillonite in ScCO<sub>2</sub> condition

**Authors:** Kaiyuan Mei<sup>None</sup> ; Liwei Zhang<sup>1</sup> ; Yan Wang<sup>None</sup> ; Manguang Gan<sup>None</sup> ; Xiaojuan Fu<sup>None</sup> ; Quan Xue<sup>None</sup>

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ScCO<sub>2</sub> was used as the solvent and intercalator when micro crystallized Ca-montmorillonite(MC Ca-MMT) was modified from Ca-MMT powder. With micro crystallization, carbonates crystallite was produced between Ca-MMT layers and provided active sites for the further reaction when mixed with oilwell cement. Enhanced oilwell cement by MC Ca-MMT was investigated based on the mechanical property and microstructure variations after curing in accelerated carbonation conditions. The microstructure of carbonation layers in enhanced oil well cement was observed and calculated according to the CT scanning results.

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## Mineral reaction and salt precipitation on a chip: understanding aquifer-relevant geological processes during CO<sub>2</sub> injection

**Authors:** Tiancheng Ji<sup>1</sup> ; Peixue Jiang<sup>1</sup> ; Ruina Xu<sup>1</sup>

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Geologic CO<sub>2</sub> sequestration into deep saline aquifers is one strategy to reduce global atmospheric CO<sub>2</sub> levels. Injectivity plays a key role in determining the storage capacity of aquifers. During CO<sub>2</sub> injection into an aquifer, acid dissolution of carbonates arises due to CO<sub>2</sub>-acidification of formation water, enhancing permeability and connectivity. While salt precipitation within the brine-saturated porous media occurs as saline water is evaporated by injected CO<sub>2</sub>, severely reducing aquifer porosity and permeability. In turn, changes in pore structure and surface composition resulted from geochemical reaction and salt precipitation will alter the porosity, permeability and capillary pressure for the two-phase flow, changing the phase distribution of CO<sub>2</sub> and saline. Understanding the interaction of mineral reaction, salt precipitation and multiphase flow on the pore-scale is essential in order to assess and optimize carbon sequestration efforts.

To date, there have been a number of pore-scale experimental studies concerning mineral reaction or salt precipitation. While these various experimental studies can provide some insight into mineral precipitation and dissolution kinetics or salt precipitation dynamics, most of them are conducted at ambient conditions, which are not representative of real reservoir conditions. Moreover, few studies consider the complex interplay of mineral reaction, salt precipitation and two-phase flow.

In this paper, pore-scale visualization experiment containing CO<sub>2</sub>-water two-phase flow, geochemical reaction and salt precipitation has been conducted at typical formation temperature and pressure. A micromodel with real rock structure coated by calcium carbonate (CaCO<sub>3</sub>) and saturated with brine is used to resemble the saline aquifer composed of quartz and carbonate.

The functionalization of micromodels with CaCO<sub>3</sub> is accomplished by treating the glass micromodel with silane coupling agent and then alternately pumping CaCl<sub>2</sub> and Na<sub>2</sub>CO<sub>3</sub> solution into it. Raman spectroscopy and optical microscope are used to characterize coated micromodels. These results verify that the inner surface of the micromodel is covered with calcite particles of about 5-8 micrometers in size, and its hydrophilicity is enhanced compared with the original glass surface.

Then, the brine-filled micromodel is mounted on an inverted optical microscope to visualize the dynamic drainage processes using CO<sub>2</sub> of different flow rate at different temperature and pressure. SEM imaging is applied to analyze the resulting mineral and salt. We find that low CO<sub>2</sub> flow rate results in dissolution of CaCO<sub>3</sub> and salt accumulation occurs as there is enough time for ions to diffuse. Increasing the CO<sub>2</sub> flow rate can suppress the dissolution of CaCO<sub>3</sub> and capillary reflow of brine. This result means that the geochemical reaction between saline and rock can be hindered by the evaporation effect of high flow rate of CO<sub>2</sub> near the injection well and salt blockage is suppressed. As more water evaporates into CO<sub>2</sub> as it migrates in the aquifer, rock dissolution occurs because of formation of carbonic acid.

In summary, we take new insight into interaction of mineral reaction, salt precipitation and multiphase flow at pore scale, which provides a fundamental understanding of reaction and precipitation dynamics during CO<sub>2</sub> injection and paves way for future studies related to injecting more CO<sub>2</sub> in aquifers.

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MS1 / 748

## **Mineralisation from carbon dioxide convective dissolution in a packed bed Hele-Shaw reactor**

**Authors:** Delora Gaskins<sup>1</sup> ; Sam Dehaeck<sup>None</sup> ; Anne De Wit<sup>2</sup>

<sup>1</sup> *Université Libre de Bruxelles*

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Pilot projects to sequester CO<sub>2</sub> in geologic formations as part of Carbon Capture and Sequestration (CCS) efforts to mitigate anthropogenic climate change have obtained evidence of the mineralization of injected CO<sub>2</sub>. Basalt aquifers like in CarbFix and the Wallula Basalt Pilot Project contain minerals like olivine which can liberate ions to mineralize and deposit the carbonates as they themselves dissolve. Flow through experiments in olivine show evidence for dual control of carbonation by reactive and transport processes 1 and the modification of the permeability of the host rock [2]. We have investigated the impact of porosity and permeability changes on the spatiotemporal dynamics of mineralization of calcium carbonate formed from the convective dissolution of carbon dioxide. We report our experimental study of convective dissolution of carbon dioxide in a modified vertical Hele-Shaw cell where the carbon dioxide is dissolved into host solutions of different concentrations of dissolved portlandite (Ca(OH)<sub>2</sub>) which reacts to form solid CaCO<sub>3</sub>. For the modification of the cell, glass beads of different diameters were packed into the cell in order to vary the porosity and permeability. We show that the precipitation front advances more slowly for the smaller beads as well as for the higher concentrations of reactant.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

1. Peuble, S. et al. CO<sub>2</sub> geological storage in olivine rich basaltic aquifers: New insights from reactive-percolation experiments. *Appl. Geochemistry* 52, 174–190 (2015).
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MS6-A / 709

## Modeling capillary fluctuations for fluid flow with lattice Boltzmann methods using LBPM

**Authors:** Ming Fan<sup>1</sup> ; James McClure<sup>1</sup> ; Steffen Berg<sup>2</sup> ; Ryan Armstrong<sup>3</sup>

<sup>1</sup> *Virginia Tech*

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Capillary phenomena have important consequences for fluid flow in geological systems, with relevant applications including carbon sequestration, recovery of oil and gas, and management of water resources. In capillary dominated systems where multiple length scales are present, accompanying timescales will also arise when considering the system dynamics. In these systems, the available thermal energy is insufficient to overcome internal energy barriers, which inhibits mixing and prevents the system from exploring all possible micro-states within the timescale of interest. Multiscale fluctuation terms arise in the non-equilibrium energy dynamics due to spatial and temporal deviations associated with intensive thermodynamic variables. How to characterize and interpret these fluctuations has been a long-standing problem for immiscible fluid flow in porous media.

In this study, 3D pore structure extracted from micro-CT images of Bentheimer sandstone were used to define interior boundary conditions of flow modeling in a pore-scale lattice Boltzmann simulator, LBPM, to simulate multiphase flow within the pore space. LBPM is an open source software package

that has been developed to simulate fluid flows through porous media (McClure et al. 2020). Non-equilibrium thermodynamic equations for immiscible fluid flow in porous media were derived using time-and-space averaging (McClure et al. 2021). In the context of this theory, capillary fluctuation terms are assessed during steady-state displacement. We investigate the influence of representative elementary volume (REV) effect on capillary fluctuations that are due to typical pore-scale events for drainage and imbibition process in porous media. The results indicate that capillary fluctuations are an essential consideration to determine REV for immiscible fluid flow.

Reference:

McClure, J. E., Li, Z., Berrill, M., & Ramstad, T. (2020). The LBPM software package for simulating multiphase flow on digital images of porous rocks. *Computational Geosciences*, 1-25.

McClure, J. E., Berg, S., & Armstrong, R. T. (2021). Capillary fluctuations and energy dynamics for flow in porous media. arXiv preprint arXiv:2012.09206.

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MS19 / 80

## Modeling coupled porous media/free flow/drop interaction in a PEM fuel cell using a pore-network approach

**Authors:** Cynthia Michalkowski<sup>None</sup> ; Veronika Schleper<sup>None</sup> ; Rainer Helmig<sup>1</sup>

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A sophisticated water management is crucial for improved operating conditions of a polymer electrolyte membrane fuel cell (PEM FC). Therefore, it is necessary to understand the transport mechanisms of water throughout the cell constituents, where the an intelligent use and drainage of the water buffer can be used to enhance performance of the fuel cell. Microscale modeling of diffusion layers and gas distributor has been established as a favorable technique to investigate the ongoing processes.

Investigating the interface between the GDL and gas distributor, a particular challenge is the combination and interaction of the multiphase flow in porous material of the GDL with the free flow in the gas distributor. Drops emerging from the porous domain at the interface have a strong influence on the exchange of mass, momentum and energy between the two flow regimes. Modeling drop-related processes on the pore-scale is usually computationally expensive.

In this talk, I present a computationally efficient approach to model pore-scale drop interface processes: A pore network model captures the pore-scale processes in the porous domain of the GDL. The free-flow domain of a PEM fuel cell gas distributor is reduced to a one-dimensional formulation including the coupled fluxes of the gas and liquid phases in rectangular micro-channels. For the interface, drop formation, growth and detachment are taken into account as well as transport of the components in the gas phase. The coupling of these domains allows an efficient computation of the main influencing phenomena on the pore-scale at the interface between porous medium and channel flow.

I investigate the influence of the reactions and production rates of water in the fuel cell on the interface processes between GDL and gas distributor. In a first scenario, the detached droplets are assumed to be transported away by the gas flux in the channels. In a second scenario, the detached droplets form a liquid film at the channel wall with a saturation dependent transmissibility for both phases.

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## Modeling lithium diffusion in battery cathodes considering chemo-mechanically induced damage

**Authors:** Jeffery Allen<sup>1</sup>; Peter Weddle<sup>1</sup>; Ankit Verma<sup>1</sup>; Anudeep Mallarapu<sup>1</sup>; Francois Usseglio-Viretta<sup>1</sup>; Donal Finegan<sup>1</sup>; Andrew Colclasure<sup>1</sup>; Volker Schmidt<sup>2</sup>; Orkun Furat<sup>3</sup>; David Diercks<sup>4</sup>; Kandler Smith<sup>5</sup>

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This talk will present a 3D, continuum-level damage model for simulating Lithium diffusion within generated  $\text{Li}_x\text{Ni}_{0.5}\text{Mn}_{0.3}\text{Co}_{0.2}$  (NMC 532) secondary cathode particles. The primary motivation of the particle-level model is to inform cathode-particle design and determine charging profiles that reduce cathode fracture. The model considers NMC 532 secondary particles containing an agglomeration of anisotropic, randomly oriented grains. The model predicts that secondary-particle fracture is primarily due to non-ideal grain interactions with slight dependence on high-rate charge demands. The model predicts that small secondary-particles with large grains develop significantly less damage than larger secondary particles with small grains. Finally, the model predicts most of the chemo-mechanical damage accumulates in the first high-rate cycles. This chemo-mechanical “damage saturation” effect indicates that initial secondary-particle fracture occurs within the first few cycles, while long-term cathode degradation is not solely chemo-mechanically induced.

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## Modeling of the droplets capture/release dynamic of Water-Alternated-Emulsion flooding in porous media through a non-equilibrium mass transfer.

**Authors:** Fabian Andres Tapias Hernandez<sup>1</sup>; Ranena V. Ponce F.<sup>2</sup>; Marcio Carvalho<sup>2</sup>; Rafael Valladares de Almeida<sup>3</sup>

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Water-alternated-emulsion (WAE) injection is an alternative chemical enhanced oil recovery method (cEOR) that improves water mobility control and sweep efficiency flow diversion. When injected, the dispersed phase of stable diluted oil-in-water (O/W) emulsions flow as conformance agents towards the thief or high permeable porous media zones blocking the preferential flow paths by different entrapment mechanisms, diverting the chased water front to upswept zones. This method is promissory in the Brazilian pre-salt oilfields since seawater along with produced water might be conditioned in the offshore petroleum platforms and re-injected in the reservoir reducing logistic costs as well as weight and space constraints typically high in comparison with other cEOR methods such as polymer or surfactant injection.

Indeed, the execution of a pilot test of some enhanced oil recovery method requires previous assessment at laboratory scale and subsequent reservoir upscaled results as part of a decision-making process that includes uncertainties analysis through numerical simulation. To properly model complex phenomena, as emulsion flow in porous media, representing the physical-chemical-mechanical coupling mechanisms occurring at the microscale and their correlation with the macroscopic effect is challenging. Inherent characteristics of the injected emulsion and porous media, such as drop-to-throat size ratio, impacts the emulsion flow and performance as water mobility control agent. Several models intend to represent and forecast emulsion flow through porous media, however, there is a lack in the understanding and modeling the fundamental physical phenomena occurring at pore scale, i.e., drop capture and release mechanisms, and its upscaling to macro-scale through a reservoir simulation software is still rather vague.

This work encompasses the modeling of straining, interception, release and re-entrainment droplets phenomena through nonequilibrium mass transfer equations. Furthermore, it incorporates parameters as emulsion viscosity, rock permeability reduction due to oil drops retained concentration, and blockage effects on the WAE performance. This approach was validated through the history matching of the WAE core flooding experiments at low capillary numbers. The differential equations were solved using Thermal & Advanced Processes Simulator - STARS - from Computed Modelling Group - CMG.

The numerical approach demonstrates the improvement of the history matching of the experimental data by using three kinetic reactions that represent the non-equilibrium mass transfer between oil drops component to the rock surface. In this model, the emulsion mobility control and sweep efficiency effects are accounted through permeability changes, which are updated according to the emulsion concentration retained in the porous media. The results enable easier upscaling, already coupling with a reservoir simulation software, for future numerical assessment and forecasting of WAE in reservoir models.

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## Modeling on contaminants removal by foam with nanoparticles in heterogeneous porous media

**Authors:** Qingjian Li<sup>1</sup> ; Valentina Prigiobbe<sup>1</sup>

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Bubbles dispersed into a liquid phase create a wet foam, which is a complex fluid with a volume fraction of the gas phase up to 97 vol.%. It controls the flow front by the Jamin Effect and directs the fluid into areas that were previously difficult to reach by water or gas. Nanoparticles have been used to stabilize bubbles. They can adsorb at the gas-liquid interface providing enhanced stability to the foam and moving with foam. This process opens the opportunity for the foam to deliver the nanoparticles in heterogeneous porous media to overcome challenges like viscous fingering, inhibited sweep, etc. Application is, e.g., in the remediation of contaminated sites. There are few worked in the literature focused on reactive nanoparticle transport in porous media with bubbles and at the current stage transport models cannot describe the system as the mechanisms of particle-particle and particle-bubble interaction during transport are not well understood, yet.

Here, a modeling work focusing on removing contaminants from 2D heterogeneous porous media by foam with reactive nanoparticles is presented. Upon previous experimental studies, the transition between weak foam and strong foam has been incorporated to describe different foamability of surfactants. Also, constitutive equations for degradation, attachment/detachment, straining, and agglomeration were accounted for in the model. It was observed that the distribution of nanoparticles could be significantly enhanced by the foam and reaching low permeability zones. The remediation period is reduced compared with nano-remediation and the back diffusion phenomena were prohibited. From the prospective of an environmental engineering application in nano-remediation, this work suggests that foam can be a valuable alternative to conventional methods to deliver nanoparticles in the subsurface in an efficient and sustainable manner, given the negligible amount of water required.

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Poster + / 59

## Modeling rate-dependent relative permeability of three-dimensional heterogeneous structures with a one-dimensional semi-analytical approach

**Authors:** Ziv Moreno<sup>1</sup> ; Avinoam Rabinovich<sup>2</sup>

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Investigation of multi-phase flow in heterogeneous porous media is important for several fields, including enhanced oil recovery, CO<sub>2</sub> storage in geological formations, and groundwater contaminant treatment. One of the key properties in characterizing such flows is phase permeability and its dependence on saturation, i.e. relative permeability curves. Such properties are usually determined via coreflooding experiments, where core samples are injected with several fluids at altering fractional flows. However, due to heterogeneity, the core's effective relative permeability curves change with the injection rate. Thus, full characterization requires conducting a significant number of coreflooding experiments with altering injection rates and fractional flows, which is a complex and time-consuming process.

The following work presents a novel framework for evaluating relative permeability curves at altering injection rates from a single injection-rate coreflooding experiment. A one-dimensional semi-analytical solution to two-phase flow at steady state is used to obtain profiles of the saturation, capillary pressure, and overall phase pressure gradient. The one-dimensional permeability profile is calibrated by matching the semi-analytical model to slice average saturation values, obtained from three-dimensional measurements, and the overall wetting phase pressure gradient. Once calibrated, the permeability profile is implemented in the semi-analytical model to estimate the effective phase

relative permeability curves at varying injection rates. This method was tested and validated on three different scenarios: two synthetic cases with different permeability fields, and one case of realistic data based on coreflooding experiments conducted on a sandstone “Shezaf” rock sample. Results have shown that the proposed approach is capable of capturing the effective relative permeability of both phases, for all of the tested scenarios, at all injection rates, by calibrating the one-dimensional permeability profile to a single total injection rate including four fractional flows. In addition, it was found that the harmonic mean of the one-dimensional permeability profile is in a good agreement with the core’s effective permeability, thus setting an additional validation of the obtained one-dimensional permeability profile.

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MS8 / 622

## Modeling the evolution of fractured media using a multiscale approach

**Authors:** Sergi Molins<sup>1</sup> ; David Trebotich<sup>1</sup> ; Carl Steefel<sup>1</sup>

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Understanding the evolution of fractured media is essential in many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO<sub>2</sub> sequestration, nuclear waste storage, and geothermal energy extraction. This evolution is the result of coupled flow, transport, reaction and geomechanical processes and is affected by both the physical and mineralogical heterogeneity of fractured media.

Here we focus on the geochemically driven evolution of fractured media and the role of transport processes. In the fracture opening, the transport of solutes is determined by the dynamics of flow in the complex geometry of the fracture. In the matrix bordering the fracture, reactions with the solid phase and solute transport through the porous medium are affected by the heterogeneity in the mineralogical composition of the matrix and in the porous medium properties. The evolution brought on by the dissolution-precipitation reactions may result in further enhancement of this heterogeneity. This includes the development of an altered layer in the matrix bordering the fracture, with heterogeneous porosity, tortuosity and permeability, and widening/narrowing of the fracture opening.

In this work, we develop a model of fracture evolution that conceptualizes the fractured medium as a multiscale medium composed of a fracture (or fractures) and a porous matrix. Fracture processes are described with a pore-scale model, while matrix processes are described with a porous medium model. The model is implemented in the Chombo-Crunch reactive transport code (Molins et al. 2012; Trebotich et al. 2014; Molins et al. 2014, 2017, 2019, 2020). We use this model to simulate CO<sub>2</sub> attack on fractured cementitious media. The geochemical problem follows from experimental and modeling work by (Li, Steefel, and Jun 2017). Flow of a CO<sub>2</sub>-rich solution in the fracture is followed by the alteration of the cementitious matrix as the invading solution diffuses into the matrix. Both precipitation and dissolution reactions take place resulting in increases and decreases in porosity locally. In contrast to previous work, consideration of flow and transport processes in the fracture (both over its width and along its length) makes it possible to capture the heterogeneous evolution of the matrix not only in the direction perpendicular to the fracture but also parallel to the fracture.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

Li, Qingyun, Carl I. Steefel, and Young-Shin Jun. 2017. "Incorporating Nanoscale Effects into a Continuum-Scale Reactive Transport Model for CO<sub>2</sub>-Deteriorated Cement." <https://doi.org/10.1021/acs.est.7b00594>.

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MS9 / 480

## Modeling the force balance controlling spatial distribution of deposited polymeric substances in porous media

**Authors:** Peter Lehmann<sup>1</sup> ; Pascal Benard<sup>1</sup> ; Mohsen Zare<sup>2</sup> ; Andrea Carminati<sup>1</sup>

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Plant roots and bacteria alter the soil physical properties by releasing a polymeric blend of substances (e.g. extracellular polymeric substances and mucilage). Despite experimental evidence of the impact of such polymer solutions on water fluxes across the root zone, the physical mechanisms controlling the spatial distribution in complex porous media (soils) have not yet been addressed. In particular, it is not clear how the physical properties of polymer solutions (viscosity, surface tension and water adsorption, all depending on the polymer concentration) shape the configuration of the liquid phase in porous media. In this study, we present a new approach by modeling the (polymer concentration dependent) force balance between viscous flow and water adsorption, defining a threshold for the immobilization of the polymeric network. At this critical point, the polymers are deposited as two-dimensional surfaces, such as hollow cylinders or interconnected surfaces. We implement this force balance in three-dimensional simulations of drying in porous media to determine the polymer deposition at the critical point. Simulations are conducted for different drying rates, polymer concentrations and particle size distributions. Simulations are compared with results of scanning electron microscope and X-ray imaging to improve our understanding of the rules defining the polymer deposition.

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MS6-A / 127

## Modeling transport of methane under nanoconfinement and in complex geometries using LBM

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Transport of shale gas is in general a multiscale process: gas flows through the matrix, which is mainly composed of nano-size (microscale) pores, followed by a fracture network, and eventually into a wellbore. Accurate prediction of flow behavior in the shale matrix is critical for efficient development of shale gas reservoirs. Current continuum-based approaches may not be appropriate to simulate transport in microscale pores. On the other hand, molecular dynamics (MD) simulations are capable of capturing the relevant microscale physics with high fidelity, albeit at a substantial computational cost, which restricts MD simulation to rather small systems and computational domains. This limitation creates a gap between the continuum-based models and MD simulations. The lattice Boltzmann method (LBM) is a suitable candidate to bridge this gap. In this work, the multiple-relaxation-time (MRT)-LBM is used to study methane transport in nano-size pores. Adsorption effects near solid boundaries, as well as non-ideal behavior of fluids, are accounted for via incorporating appropriate force terms in LBM. Parameters associated with the force terms in the equation of state (EOS) are studied in detail and their optimum values are proposed. Simulation results obtained using LBM are validated against those from MD predictions. Results show that LBM captures slip velocity and nonuniform distribution of density predicted by MD simulations. This motivates the use of LBM in scale translation of the physics of mass transport in complex permeable media.

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## Modelling Multi-scale 3-D Digital Rocks by a New Image Segmentation Method

**Author:** Jingxu Yan<sup>1</sup>

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Conventional digital rocks constructed by micro-CT with single resolution cannot identify entire pore space and mineral components of tight sandstones due to the multi-scale pores and high clay contents. The porosities of digital rocks are far less than those measured in lab, which results in the difference between measured petrophysical properties and calculated properties based on digital rocks. In this study, we proposed a method to construct multi-scale digital rocks by fusing 3-D images scanned via micro-CT at different resolutions. First, cylindrical tight sandstone samples with a diameter of 25.4mm were scanned at a resolution of 13.99 $\mu$ m to construct low-resolution 3-D grayscale images. Then, sub-plugs with a diameter of 5mm were drilled from the cylindrical samples and scanned by micro-CT at a resolution of 2.99 $\mu$ m to build high-resolution 3-D grayscale images. Furthermore, the two grayscale images were precisely registered using SIFT image registration method. In case of high-resolution images, watershed segmentation algorithm was applied to segment the cores into pores and minerals. The relationship curves between grayscale value and composition of the low-resolution grayscale images were established based on the registered region. A multi-scale digital rock was built from the low-resolution grayscale image after segmentation. The fine intragranular pores that cannot be resolved by the high-resolution images are acquired by board ion beam scanning electron microscope (BIB-SEM). The bulk porosities of multi-scale digital rocks agree well the helium porosity measured in lab. The effective elastic moduli of each voxel are determined by its mineral composition and fine structure. Given the effective bulk and shear moduli of each voxel, the elastic modulus of the rock can be calculated using the finite element method (FEM) based on the low-resolution digital rocks. The predicted elastic moduli match the measured results well. The numerical results show that the modeling method provides an accurate digital rock that can represent true tight sandstones in porosity and mineral components.

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MS25 / 145

## **Modelling and analysis of multicomponent transport at the interface between free and porous-medium flow influenced by radiation and roughness**

**Authors:** Rainer Helmig<sup>1</sup> ; Katharina Heck<sup>2</sup> ; Edward Coltman<sup>1</sup>

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Evaporation of water from a partly saturated porous medium is an important process. Evaporation fluxes contribute to the water budget and play a role in the energy balance at the soil surface. It is therefore an important component in the hydrological cycle. Moreover, evaporation is also the driving process of soil salinization.

The focus of this presentation will be to analyse multicomponent transport between a porous medium and a free flow. Furthermore, radiation is included in the coupling conditions of the two domains, which makes it possible to evaluate the effect of a diurnal cycle of radiation on evaporation and the transport of other gaseous components. This is highly relevant for predicting greenhouse gas emissions and evaporation rates under natural conditions from soil.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

K. Heck, E. Coltman, J. Schneider, and R. Helmig. Influence of radiation on evaporation rates: A numerical analysis. *Water Resources Research*, 56(10), 2020. **Acceptance of Terms and Conditions:**

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**MS6-B / 249**

## Modelling dynamic behavior of an infiltration trenches system

**Author:** Marco Berardi<sup>1</sup>

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This study takes a cue from the research and monitoring activities held in an infiltration trenches cluster downstream of a wastewater treatment plant in Castellana Grotte (Puglia).

Simply using mass balance arguments and Darcy's law, we model the variation in time of hydraulic head in the infiltration trenches: as a result of this modelling, the saturated hydraulic conductivities are estimated. Such head levels are also monitored, together with the total daily water inflow to the trenches; the water flowing through the permeable septa that separate adjacent trenches, as well as infiltration towards external walls of the trenches cluster are modelled by a ODEs system: such model takes into account both anisotropy factors and differences in altitude among the trenches.

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**MS17 / 350**

## Modelling hydrate formation in porous media: Capillary inhibition effects

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Marine sediments hosting methane hydrates (MH) cover pore sizes ranging from coarse-grained sands to fine-grained silts and clays. Coarse-grained sediments favour methane gas and methane saturated water flow and hence the formation of large concentrations of MH in pores (~60-90%) (e.g., Weinberger and Brown, 2006). However, most of the world's MH inventory exists disseminated within fine-grained sediments in very low saturations (below 10%) (e.g., Max et al., 2016). Experimental tests (e.g., Anderson et al., 2009; Chuvilin et al., 2005; Handa and Stupin, 1992; Østergaard et al., 2002; Uchida et al., 1999, 2004) and theoretical models (e.g., Clennell et al., 1999; Henry et al., 1999; Sun and Duan, 2007) have evidenced that MH confined in narrow pores (<100 nm) are subjected to capillary effects that disturb their thermodynamic stability. These studies show that capillary pressure hinders MH stability by decreasing the pore water activity and increasing aqueous methane solubility. Then, as pore size decreases, capillarity effects shift the MH equilibrium phase boundary towards higher pressures and/or lower temperatures than those predicted from bulk conditions (no sediment); similar and in addition to the shift generated by chemical inhibitors like salt. Understanding the stability conditions of natural MH is critical for a reliable prediction of the methane budget stored in hydrate systems as well as to assess the feasibility of its extraction for energy purposes (Ruppel and Waite 2020). Here, we first propose an equilibrium model to simulate MH formation conditions accounting for capillary effects. Analogously to water freezing behaviour in pores (e.g., Nishimura et al., 2009), our model assumes MH formation to be controlled by the sediment pore-size distribution and the balance of the capillary forces developed at the liquid-hydrate interface. Our model uses the Clausius-Clapeyron relation for the thermodynamic equilibrium of methane and water chemical potentials in hydrate systems. It defines the thermodynamic equilibrium conditions that need to be satisfied by the liquid and MH phase pressures and the system temperature in a single pore size. Our model captures the depression of the MH equilibrium temperature observed experimentally during hydrate formation/dissociation tests performed in narrow pores ( $\leq 30.6$  nm) (e.g., Deaton and Frost, 1946; Jhaveri and Robinson, 1965; McLeod and Campbell, 1961; Østergaard et al., 2002; Anderson et al. 2003, Anderson et al. 2009). Then, the model is combined with van Genuchten's capillary pressure (van Genuchten, 1980) to relate the thermodynamic properties of the hydrate system to the host sediment pore-size distribution. The model is finally applied to simulate and quantify MH formation in sand, silt and clays with different content of fine-particles, under equilibrium conditions and without mass transfer limitations. The simulations evidence that capillary effects are negligible in sand and almost negligible in silty sediments but exert a key control in MH stability and saturation within clayey sediments. In particular, the results show that at thermodynamic conditions typically found in the seabed, capillary effects may reduce the maximum hydrate saturation expected in sediments with a high content of fines up to 50%.

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## **Modelling pressure-saturation curves that exhibit hysteresis and forced imbibition with the pore-morphology method**

**Authors:** Christian Hinz<sup>1</sup> ; Andreas Wiegmann<sup>1</sup> ; Sven Linden<sup>1</sup> ; Jens-Oliver Schwarz<sup>1</sup>

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The key to accelerate research and production in the energy industry resides in the efficient and generally applicable modelling of two-phase flow at the pore-scale. Here, we present the capabilities of the pore-morphology method (PMM) that we developed during the past two decades and our recent advancements.

The PMM was originally introduced in 2001 by Hilpert and Miller to model the pressure-saturation curves of a drainage process based on 3D scans of the micro-structure of a porous medium, for example  $\mu$ CT images of rocks. Since then, the PMM has found its place somewhere between pore-network models (PNM) and direct numerical simulations (DNS), frequently using the Lattice Boltzmann method. PMM combines the geometric analysis of the pore space to distribute the two fluid phases (as does PNM) with a direct numerical simulation on the original micro-structure (as does DNS), albeit only considering single-phase flows.

In 2005, Schulz, Becker and Wiegmann added the capability to compute relative permeabilities to the PMM by running single phase flow simulations on either of the two phases. Later, Becker et al. enhanced the PMM to model also imbibition and residual phases, and added entry pressure artefacts. Additionally, the flow solver was changed from a Lattice Boltzmann implementation (ParPaC) to a FFT-based implementation (FFF-Stokes, EJ-Stokes, SIMPLE-FFT) and to an adaptive grid-based implementation (LIR). In 2014, Schulz et al. introduced varying contact angles into the PMM. The

changes in the flow solver resulted in only small changes to the solution because: (a) the implementation of boundary conditions is slightly different between collocated and staggered grids (ParPaC vs. SIMPLE-FFT and LIR), (b) the grid-coarsening produces different systems of equations (SIMPLE-FFT vs. LIR), and (c) the stopping criteria can be reached by different paths even for the same discretization as the solution method changes, and all solvers are iterative in nature. Changing the flow solvers has had however a remarkable impact in decreasing run-times and memory requirements. A good example for this is the use of velocity- and pressure-fields from simulations with a similar saturation as initial guesses for the next simulation.

For all that, a higher impact comes from modifying the algorithms that distribute the phases in the micro-structure. In this spirit, this presentation will show how the PMM can be extended to model hysteresis and forced imbibition and, so, create more complex and real pressure-saturation curves than previous versions of the PMM.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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MS2 / 711

## Modelling rhizosphere water movement in whole plant models

**Authors:** Daniel Leitner<sup>1</sup> ; Andrea Schnepf<sup>2</sup> ; Jan Vanderborgh<sup>None</sup> ; Harry Vereecken<sup>None</sup>

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Plant productivity is directly influenced by water and nutrient uptake. Therefore, functional-structural root models need to accurately describe rhizosphere processes. Such models will enable better agricultural management strategies and improved root trait selection for plant breeding. Due to their complexity functional-structural root models are hard to analyse. In Schnepf et al. (2020) various research groups developed a systematic framework for benchmarking individual root functional models and their individual components. In this work we will focus on root water uptake and how appropriate sink terms can be developed in macroscopic (plot-scale) models.

Macroscopic water movement is commonly described by the Richards equation and the impact of root water uptake is described by a sink term. The sink term is either derived by some averaging or homogenisation procedure or by equations based on empirical observations. Common choices are to set the sink term proportional to the root surface density, or to use line sources which represent the root architecture. In Schnepf et al. (2020) various sink terms were benchmarked and compared to an exact 3-dimensional solution of a small root system, where a mesh was calculated and refined towards the root surface. Results showed that local water depletion in the rhizosphere will affect total water uptake when the soil is sufficiently dry.

A solution to this problem was presented by Mai et al. (2019) who described the rhizosphere by a 1-dimensional model around each root segment. The 1-dimensional grid was refined at the root surface enabling an accurate representation of the plant-soil interface. In the following we describe and generalize the coupling steps, especially with a focus on the point of contacts between the different sub models (see Figure 1). The evolving root architecture is described by CPlantBox (Schnepf et al, 2018), macroscopic water movement as well as water movement in the 1D rhizosphere models are calculated in DuMux (Flemisch et al. 2011, Koch et al. 2020).

Using 1d-cylindrical models to describe the plant rhizosphere is a promising approach for development of better functional-structural root models. It enables us to separately develop and analyse the microscopic rhizosphere models. Such models can be directly used in the proposed coupling framework, where no additional upscaling is needed. This enables an analysis how changes of microscopic parameters will affect the macroscopic results.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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## Modelling the role of vWF in initiating arterial thrombosis

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Coronary heart disease is characterised by the formation of plaque on artery walls, restricting blood flow. If a plaque deposit ruptures, blood clot formation (thrombosis) rapidly occurs with the potential to fatally occlude the vessel within minutes. Von Willebrand Factor (vWF) is a shear-sensitive protein which has a critical role in blood clot formation in arteries 1. At the high shear rates typical in arterial constrictions (stenoses), vWF undergoes a conformation change, unfolding and exposing binding sites and facilitating rapid platelet deposition.

We develop a continuum model for the initiation of thrombus formation by vWF in an idealised arterial stenosis. We extend current continuum models for thrombosis by explicitly modelling the vWF unfolding dynamics [2,3]. The vWF and platelets are split into free and bound populations, where the bound populations are fixed to the stenosis surface and the free populations, are advected with

the fluid. The model for vWF extension in the flow is derived by considering a dilute limit of a non-linear viscoelastic fluid model, the FENE-P model, such that the protein has a negligible contribution to the fluid viscosity but the influence of fluid shear on protein extension is retained.

We exploit the slow timescale of thrombosis initiation to construct a reduced model of thrombosis, this allows us to examine the role of vWF in the cascade prior to rapid thrombus growth and vessel occlusion. We consider free vWF binding to available collagen on the stenosis surface which then forms a base for platelet deposition. Free platelets are then able to deposit to the bound vWF with a variable binding rate which increases proportional to the length of vWF.

Through numerical simulations, we investigate the effect of varying stenosis geometry and blood flow conditions on the unfolding of vWF and subsequent platelet binding. This allows prediction of the location and timescale platelet deposition for a given stenosis.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## **Modification method and adaptability of fluid phase states in nanopores**

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With the development of massive gas injection in shale and tight reservoirs, the multiphase behavior of nanoscale pores before and after gas injection has attracted increasing attention. A large number of published literature have shown that due to wall adsorption and capillary forces, the phase behavior of fluids in micro and nano pores is significantly different from that of conventional reservoirs, such as phase transformation hysteresis. The existing equations of state, especially the PR-EOS method used to calculate the gas-liquid equilibrium, cannot accurately describe the changes of the gas-liquid state in the nanopore. Therefore, it is necessary to modify the EOS equation according to the relevant terms introduced in the corresponding nanopore phase state mechanism or in combination with other methods. Three kinds of correction methods for phase state calculation in nanoscale pores are emphatically discussed, including: modifying the molar volume in the equation of state; The capillary force of micro-nano channel is considered. Consider changes in critical parameters. While this document is the method in the nanoscale pore in order to improve the EOS model in the prediction of the precision of phase behavior change as the result, but in the case of a given component simulation, in the process of gas injection, the component concentration changes, the existing EOS correction method is adaptive to varying component is each part of the unknown, the lack of mutual relationship between each correction method. This paper intends to evaluate the accuracy of the three correction methods through the experimental data in the literature, and the results show that the combination of the three correction methods cannot accurately reflect the change of phase state, which indicates that there is mutual interference among the correction methods.

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## Modification of Darcy's Law by Considering the inertial effect

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Permeability is a parameter introduced by Darcy's Law, which is believed to be an intrinsic property of the porous medium and should be independent of the nature of the fluid flowing through it. However, Darcy's Law has specific conditions. The assumptions inherent to Darcy's law are (1) a single, incompressible fluid is flowing; (2) flow is in the laminar regime; (3) the fluid is immobile at the pore walls; (4) isothermal conditions exist; (5) the fluid and medium are nonreactive. In this study, isothermal and nonreactive flow is considered. The dimensionless numbers corresponding to condition (1), (2) and (3) are Mach number (Ma), Reynolds number (Re) and Knudsen number (Kn) respectively. Only two of these three dimensionless numbers are independent since they are connected by  $Kn = \frac{Ma}{Re} \sqrt{\frac{\pi}{2}}$ . Therefore, and can be chosen as conditions for the establishment of Darcy's Law when isothermal and nonreactive flow is considered, where represents the gas slip effect and represents the inertial effect.

The inertial effect is studied by many researchers. The most famous and successful model is proposed by Forchheimer, which is expressed in 1D by  $\frac{dp}{dx} = -(\frac{\mu}{\kappa}V + \beta\rho V^2)$ , where  $\frac{dp}{dx}$  is pressure gradient which is imposed on the both ends of porous medium,  $\mu$  is dynamic viscosity of fluid,  $\kappa$  is intrinsic permeability of porous medium,  $\rho$  is density of fluid,  $V$  is Darcy velocity of fluid and  $\beta$  is Forchheimer coefficient. Except this, some researchers argued that the cubic term of Darcy velocity,  $V^3$ , or the n-th power,  $V^n$ , should be included in the expression rather than the squared term. All of them have a similar coefficient as Forchheimer coefficient and the focus of related research is the expression of such coefficient. However, all of the expressions are too complicated to be applied in engineering.

In this study, we are trying to derive a concise expression of modified Darcy's Law by considering the inertial effect. The idea is to propose a suitable modified boundary condition which can account for the derivation due to the moderate inertial effect. Suitable numerical cases will be conducted and results will be carefully analyzed in order to get the suitable modified boundary condition.

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## Molecular Dynamics Study on Coal Matrix Swelling Characteristics by CO<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>-N<sub>2</sub> Mixture

**Authors:** Jinrong Cao<sup>1</sup> ; Yunfeng Liang<sup>1</sup> ; Yoshihiro Masuda<sup>1</sup> ; Ziqiu Xue<sup>2</sup> ; Toshifumi Matsuoka<sup>3</sup>

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**Background:** Coalbed methane (CBM) is an important natural gas resource of growing interest [1,2]. The injection of CO<sub>2</sub> can enhance CBM recovery, meanwhile, CO<sub>2</sub> can be stored in the coalbed layer. However, CO<sub>2</sub> may induce coal matrix swelling, and an inappropriate injection design may result in the cleat closure of the coal system [3,4]. On the other hand, N<sub>2</sub> was effective to promote CH<sub>4</sub> desorption and improve sweep efficiency [5,6]. However, the major drawback associated with N<sub>2</sub> injection is that it tends to lead to an early breakthrough. In the CBM reservoirs, the coal matrix is associated with a large number of micropores that are less than 2 nm. The swelling occurs is due to the adsorption behavior in the micropores [7,8]. Due to limitation of laboratory experiments to the gas adsorption status in the micropores, the replacement process of CH<sub>4</sub> in the coal matrix and the swelling/shrinkage mechanism of the coal matrix are poorly understood.

**Methods:** In this paper, we studied the CH<sub>4</sub> recovery process by injecting CO<sub>2</sub>, N<sub>2</sub>, or CO<sub>2</sub>-N<sub>2</sub> mixture into the coal matrix using molecular dynamics simulations. The relationship between the swelling of coal matrix due to the adsorption, and permeability decline due to swelling, were then discussed. A model of a coal matrix filled with CH<sub>4</sub> was constructed, and the CO<sub>2</sub> (N<sub>2</sub> or CO<sub>2</sub>-N<sub>2</sub>) molecules were added into a large-size fracture of the coal system. This system was equilibrated to investigate coal swelling and the replacement process. A long enough simulation was performed, to allow CO<sub>2</sub> (N<sub>2</sub> or CO<sub>2</sub>-N<sub>2</sub>) molecules enough time to enter the coal matrix and displace the CH<sub>4</sub> molecules.

**Findings:** The calculated recovery factors were 79.9, 54.3, and 70.5% for CO<sub>2</sub>, N<sub>2</sub>, and CO<sub>2</sub>-N<sub>2</sub> mixture injection, respectively. After equilibration, the specific volume (i.e. volume per unit mass) and thickness of the coal matrix were estimated and compared to those at the initial stage for estimation of the coal swelling. There is a swell of 12–17% in the pure liquid CO<sub>2</sub> injection. There are no swell in the pure N<sub>2</sub> case and CO<sub>2</sub>-N<sub>2</sub> mixture case, shrinkage may be observed during N<sub>2</sub> injection and negligible during the CO<sub>2</sub>-N<sub>2</sub> mixture injection. The permeability change was also estimated by using the coal matrix swell data. The swelling estimated by the specific volume for the pure CO<sub>2</sub> case is about 17%. Therefore, the estimated permeability will drop to 0.4% of the original one. The reported porosity of the actual field has some uncertainty, but, if the natural fracture porosity of 0.4% [5] was used, the cleat will be fully closed then. Apart from the micropores, the formation becomes almost impermeable. These findings agrees with previous reports [3,6,7]. In conclusion, in the case of pure liquid CO<sub>2</sub>, the permeability will reduce dramatically. For pure N<sub>2</sub>, it can be helpful to enhance the permeability. If we carefully choose the mole fraction of CO<sub>2</sub>-N<sub>2</sub> mixture, the permeability reduction may be avoided, while keeping enough high CH<sub>4</sub> recovery factor.

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## Molecular dynamics study of methane diffusion in flexible microporosity of source rock's organic matter

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Over the last decades shale gas production from deep rock formations has become increasingly important in the gas industry. This has led to thorough examinations of fluid transport properties by molecular dynamics simulations in the organic part of the porous medium, such as those found in unconventional reservoirs, so called kerogen. Most of these studies have been done by considering the microporous structure of kerogen as a rigid solid [1-3]. However, a recent study [4] has revealed that accounting for the kerogen flexibility while investigating the hydrocarbon transport in an immature kerogen matrix could play a crucial role. Flexibility can lead to a significant increase in the free volume due to the adsorption-induced swelling that increases fluid transport when the fluid loading increases, as opposed to what found in the rigid case. This study has only been performed for a few set of thermodynamics conditions and collective diffusion has not been studied yet. All this calls for the need of in-depth studies of the flexibility effects on transport properties in immature kerogen. Thus, in this work methane diffusion in kerogen for a wide range of conditions (pressure, temperature) and fluid loading is investigated. It is proven that the collective effect on fluid transport through a deformable matrix of kerogen can be neglected. It is also shown that the trend of diffusion coefficient increases via fluid loading can be well captured using free volume scaling. Furthermore, we have started studying the carbon dioxide diffusion in the kerogen matrix. These results contribute to the investigation of fluid transport properties in such microporous medium and will be extended to study transport of carbon dioxide and methane mixtures in a near future.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## Multi-parameter Screening Study on Static Properties of Nanoparticle Stabilized Supercritical CO<sub>2</sub> Foam

**Authors:** Xiakai Song<sup>1</sup> ; Dongxing Du<sup>2</sup>

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Foam technology has been widely employed for enhancing oil recovery from mature reservoirs as well as the unconventional oil reserves. Employing CO<sub>2</sub> as the foam internal phase could not only explore extra oils from reservoirs but also in the meantime store large amount of CO<sub>2</sub> in underground formations, thereby fulfill the resourceful utilization and geological storage of the greenhouse gas. The CO<sub>2</sub> foam field applications, however, may suffer from the high-temperature, high-pressure and high salinity reservoir conditions. Adding nanoparticles (NPs) in the surfactant solution has been proven an efficient technique to increase the foam stability under harsh reservoir conditions, therefore attracts wide attention from international scholars.

As a complex gas/liquid/solid system, multiple parameters contribute in a synergic way to the static properties of the NP-stabilized Supercritical CO<sub>2</sub> (ScCO<sub>2</sub>) foam. In order to obtain the optimal recipe for excellent foam performance in terms of foamability and foam stability, comprehensive parameter screening studies have been carried out in this paper on the static properties of NP-stabilized foam with help of the Orthogonal Experimental Design (OED) method. Six influential factors, including NP concentration, surfactant concentration, temperature, pressure, oil existence, salinity, have been investigated on four levels for each factor in the range of 0-0.2wt%, 0.1-0.5wt%, 20-60°C, 5.5-9.5Mpa, 0-4wt% and 0-8wt% respectively.

The experimental results show that temperature and pressure are the main factors affecting the formability of NP-stabilized ScCO<sub>2</sub> foam, and temperature is the dominant factor on the stability of the foam. When the system condition is close to the supercritical point of CO<sub>2</sub>, the foam generation height and the foam decay rate within certain period of time shows the worst behavior. While under the system conditions far from the CO<sub>2</sub> supercritical point, such as lower temperature and higher pressure, the static properties of the NP-stabilized CO<sub>2</sub> foam behave much better. Based on parameter screening results, we obtained the formula for the NP-stabilized CO<sub>2</sub> foam with satisfactory static properties, that is, NP concentration of 0.15wt% and surfactant concentration of 0.4wt% within the studied ranges of temperature, pressure, oil and salinity values. To validate the screening study method as well as the experimental technique, the obtained formula is employed to generate NP-stabilized CO<sub>2</sub> foam under two sets of conditions of temperature of 45°C & 55°C, pressure of 9.5MPa, salinity of 2.5wt%, and oil concentration of 2.5wt%. Satisfactory foamability and foam stability properties were obtained, indicating the validity of the research works.

It is expected the experimental techniques and results reported in this paper could help on the laboratory screening and optimization of foaming agent formulations under reservoir conditions, and therefore on guidance of the NP-stabilized CO<sub>2</sub> foam technology in field practices.

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## **Multi-phase flow parameters for unconsolidated reservoirs using digital rock physics**

**Authors:** Pit Arnold<sup>dNone</sup> ; Alexandru Badescu<sup>1</sup> ; Hendrik Rohler<sup>2</sup> ; Holger Ott<sup>1</sup>

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Advances in technology and computational power have led to an increased impact of digital rock physics, i.e., simulations on the rock's pore space obtained from computer tomographic imaging. Various processes can be simulated either directly on the obtained structure or on abstracted networks

in order to obtain rock and fluid properties such as relative permeability and capillary pressure saturation functions. Typically, simulation results are corroborated with experimental data obtained from routine and special core analysis programs. Compared with experiments, simulations take only a fraction of the time to perform, allowing for additional sensitivity studies with respect to, e.g., fluid configurations. In case of unconsolidated reservoirs, however, there are often no structurally intact samples available. Even if samples are available, their usage in core analysis programs is rather limited and creating subsamples for micro-CT imaging has proved to be challenging. Therefore, the information available might be limited to grain size distributions from sieving analysis, porosity measurements and MICP data. In this study, we generate digital rock models based on grain-size distributions in order to simulate relative permeability and capillary pressure saturation functions. We match the models in the frame of the available experimental data to MICP curves by varying grain sizes, shapes and grain orientation, while keeping the systems' porosity and grain size bins as boundary criteria. Our results show a high sensitivity to grain shapes rather than sizes. Subsequently, we calculate relative permeability functions based on our matched digital models. In the present cases, Digital Rock Physics on basis of synthetic rock models may be the only source of multiphase-flow parameters. Their variation with a reasonable range in wettability assumptions serve as starting point for stochastic reservoir modeling.

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## **Multi-scale dynamics of colloidal deposition and erosion in porous media**

**Author:** Navid Bizmark<sup>1</sup>

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Diverse processes—e.g., environmental pollution, groundwater remediation, oil recovery, filtration, and drug delivery—involve the transport of colloidal particles in porous media. Using confocal microscopy, we directly visualize this process *in situ* and thereby identify the fundamental mechanisms by which particles are distributed throughout a medium. At high injection pressures, hydrodynamic stresses cause particles to be continually deposited on and eroded from the solid matrix—strikingly, forcing them to be distributed throughout the entire medium. By contrast, at low injection pressures, the relative influence of erosion is suppressed, causing particles to localize near the inlet of the medium. Unexpectedly, these macroscopic distribution behaviors depend on imposed pressure in similar ways for particles of different charges, even though the pore-scale distribution of deposition is sensitive to particle charge. These results reveal how the multi-scale interactions between fluid, particles, and the solid matrix control how colloids are distributed in a porous medium.

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## Multi-scale imaging and modelling for reactive diffusion at the pore scale

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In the frame of a project aiming to develop a multi-scale imaging and modelling procedure for reactive transport in porous media, we present our first results concerning diffusion and reaction. For the problems we consider, heterogeneous reactions are dominant, meaning that the reactive part of the fluid/solid interface must be precisely described at the local scale. On the other hand, the global spatial distribution of the solid must also be precisely characterized because it determines the representativeness of the average transport properties. Multi-scale imaging techniques can provide a “low” resolution image, corresponding to a large field of view, that can be used as input for computing the average transport properties, and “high” resolution images that describe the fluid/solid interface in details. For numerical modelling we need the “low” resolution image of all the computation domain, and “high” resolution information of the zones having a strong effect on the transport, for instance zones where significant reactions take place. Acquiring a “high” resolution image of the full computation domain is not realistic, and, if an average value is not sufficient for modelling (effective reactive surface), we need a way to incorporate in a multi-scale model both “high” resolution and “low” resolution information.

We use an iterative multi-scale numerical modelling approach: After a first simulation at the “low” resolution scale (i.e. relevant for the transport at the global scale), the zones where grid refining is necessary are selected using an error estimate procedure. Local refining can then be used to complement “low” resolution image in these zones and generate finer grid to improve the quality of the results. Different approaches are explored for this refining step. They will be exposed at the end of the presentation.

To be representative, “low” resolution 3D images are generally big. This results in a large number of grid elements and computationally demanding problems to solve. To temper the computation effort, we first perform a coarsening of the initial grid. After describing the algorithm employed to build of a non-uniform Cartesian mesh, consequences of this coarsening step will be presented for a reactive diffusion problem in terms of precision of the computed effective properties and reduction of the computation costs.

Then, the refining step will be presented and the improvements obtained using different strategies will be compared.

This work is funded by EU Horizon 2020 Marie Skłodowska-Curie Actions Innovative Training Network: MULTISCALE, Multimodal and Multidimensional imaging for EngineerRING (MUMMERING), Grant Number 765604.

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## Multilayered poroelasticity interacting with Stokes flow

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We prove the existence of a weak solution to a fluid-poroelastic structure interaction problem in which the structure consists of two layers: a thin poroelastic plate layer in direct contact with Stokes flow, and a thick Biot layer sitting on top of the thin layer. In the (quasi-static) Biot layer the permeability is a nonlinear function of the fluid content. Existence of a weak solution is obtained using a constructive proof based on Rothe's method. We provide uniqueness criteria and show that the constructed weak solutions are indeed strong solutions if one assumes additional regularity. We show how this result impacts the design of drug-eluting stents for the treatment of coronary artery disease.

The presence of drug-eluting stents alters the permeability of the arterial walls and impacts advection, reaction and diffusion of anti-inflammatory drugs, such as sirolimus, into the poroelastic arterial walls. This information helps alter the design of drug-eluting stents for improved long-term efficacy. The results presented in this talk were obtained in part with Lorena Bociu, Boris Muha, Yifan Wang, and Justin Webster.

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## Multiphase imbibition dynamics in xylem-like nanoporous media

**Authors:** Olivier Vincent<sup>1</sup> ; Théo Tassin<sup>2</sup> ; Erik Huber<sup>2</sup> ; Abraham Stroock<sup>2</sup>

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We studied experimentally spontaneous water imbibition that is triggered by capillary condensation in multiscale porous media resembling the architecture of water-conducting tissues in plants (xylem). These structures couple a nanoporous layer to arrays of microchannels of varying aspect ratio. We show that the presence of the microchannels can dramatically affect the dynamics of imbibition in the nanostructure, resulting in faster dynamics globally, and in intermittent dynamics locally. We further show that these effects can be tuned not only by the choice of the geometry of the microstructure, but also by changing the filling state of the cavities (air vs. vacuum), which suggests strategies for dynamic control of the speed of imbibition.

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## Multiphysics modeling of vanadium redox flow batteries.

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Porous electrodes are an essential component of Vanadium Redox Flow Batteries (VRFBs), which are one of the most promising technologies among the energy storage systems required for the integration of the growing supply of renewable energies into the electric grid. Vanadium RFBs have been engineered for decades and currently exhibit some early commercial scale implementations. In this context, mathematical modelling offers a great opportunity for the optimization of current VRFB performance [1-5].

In this work, a two-dimensional, macroscopic, isothermal, steady-state model of a VRFB cell is presented. It incorporates comprehensive descriptions of charge transport and mass transport of ionic species in the electrolyte and membrane, as well as of the electro-chemical kinetics in the porous electrodes. The resulting model enables an extensive understanding of the coupled phenomena that take place in VRFBs, being able to predict the performance under different operating conditions and to identify the critical parameters for the optimization of the cell design.

The electrolyte properties are characterized as a function of the State of Charge (SOC) using in-house experimental data, thus providing a more accurate description of species transport. The computed ionic conductivities are corrected and compared with experimental measurements. Besides, an experimental campaign was conducted to validate the model. Polarization curves are obtained at ambient temperature varying operating conditions such as SOC and volumetric flow rate, and OCV data is obtained as a function of the battery SOC.

### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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## Multiscale Model Reduction of Thermoporoelasticity Problems in Heterogeneous and Fractured Media Using Generalized Multiscale Finite Element Method

**Authors:** Dmitry Ammosov<sup>1</sup>; Maria Vasilyeva<sup>2</sup>; Eric Chung<sup>3</sup>

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Thermoporoelasticity problem has many applications in science and engineering: geothermal energy systems, nuclear waste disposal, wellbore stability analysis, and others. However, most of the applied problems of thermoporoelasticity cannot be solved analytically. Therefore, it is essential to develop mathematical models and efficient numerical methods. The mathematical model is described by a coupled system of equations for pressure, temperature, and displacements. We consider heterogeneous and fractured media. We apply a multiscale model reduction to reduce the size of the discrete system. We use a continuous finite element method with a Discrete Fracture Model (DFM) for fine grid approximation. For coarse grid approximation, we apply the Generalized Multiscale Finite Element Method (GMsFEM). We present numerical results for two- and three-dimensional model problems in heterogeneous and fractured media. We compute errors between the multiscale solution with the fine-scale solution for different numbers of multiscale basis functions. The results demonstrate that the proposed method can provide good accuracy with a few degrees of freedom.

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MS2 / 507

## Multiscale Modeling of Direct Contact Membrane Distillation: Macroscopic Modeling and Pore Scale Modeling

**Authors:** Hesam Bazargan Harandi<sup>1</sup> ; Anahita Asadi<sup>1</sup> ; Hossein Fathi<sup>2</sup> ; Pang-Chieh Sui<sup>1</sup>

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Membrane distillation (MD) using porous hydrophobic membranes finds applications in various areas such as desalination of seawater, industrial wastewater treatment, and pharmaceutical separation of mixtures. In this study, a direct contact membrane distillation (DCMD) module with commercially available polytetrafluoroethylene (PTFE) membranes (GE-Osmonics/0.22um and MS-3010/0.45um) is investigated with a multiscale approach. A 2D macroscopic, multiphysics model considering the conservation of species, momentum, and energy has been developed in the present study to gain an understanding of the processes in such a DCMD system. Instead of empirical correlations, this study uses a microscopic model to determine the effective transport properties, including effective mass diffusivity and thermal conductivity. The flowchart of workflow, the graphical representation of the multiscale approach used in the present study, is shown in Fig. 1. As illustrated in Fig. 1, a stochastic numerical reconstruction method is first developed to generate virtual membranes based on the membrane's pore size, fiber orientation distributions and the structure data of membranes presented by the manufacturers. To compute the transport properties subsequently needed in the macroscopic model, a finite volume operator in AVIZO and a finite volume solver in OpenFOAM, are employed to perform pore-scale simulations on the reconstructed geometries. For virtual reconstructed GE-Osmonics/0.22um PTFE membrane, the effective thermal conductivity and the effective mass diffusivity in through-plane direction are determined 0.0582W/mK and 1.07e-5 m<sup>2</sup>/s, respectively, while these transport properties are calculated 0.0571W/mK and 1.13e-5 m<sup>2</sup>/s for virtual reconstructed MS-3010/0.45um PTFE membrane. It shows a good agreement between the simulation results and published data as well as empirical relations.

Fig. 1. Workflow flowchart of the multiscale approach.

With the objective to understand the effect of transport properties computed by microscopic methods in macroscopic modeling, simulation results of the present study in relation to the experimental data with previous studies are compared and realized that the average error of flux of distillate water is reduced from 10.5% and 6% found in previous studies to 7.9% and 5.3% calculated in the present study for feed inlet temperatures of 333.15 and 313.15, respectively.

Fig. 2. Comparison of flux of distillate water for experimental and predicted responses by Hwang et al. and present model for different feed inlet temperatures and inlet velocities (permeate inlet temperature of 293 K, NaCl mass fraction of 1%, GE-Osmonics/0.22um).

Furthermore, comparing two stochastically reconstructed membranes, GE-Osmonics/0.22um and MS-3010/0.45um, show that the average amount of produced freshwater in the DCMD module with MS-3010/0.45um is 24% more than produced freshwater in the DCMD module with GE-Osmonics/0.22um.

Fig. 3. Comparison of flux of distillate water for two stochastically reconstructed membranes, GE-Osmonics/0.22um and MS-3010/0.45um, for different inlet velocities (Feed inlet temperature of 333.15K permeate inlet temperature of 293K, NaCl mass fraction of 1%, Countercurrent flat sheet).

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## Multiscale Sampling for Subsurface Characterization

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The characterization of natural subsurface formations is a challenging task because of the large dimension of the stochastic space. Typically a dimensional reduction method, such as a Karhunen-Loeve expansion (KLE) needs applied to the prior distribution to make these problems computationally tractable. Due to the large variability of properties of subsurface formations (such as permeability and porosity) it may be of value to localize the sampling strategy, so that it can better capture local variability of rock properties.

In this work we introduce the concept of multiscale sampling to localize the search in the stochastic space. We work within a Bayesian framework. We combine the simplicity of a preconditioned Markov chain Monte Carlo (MCMC) method with a new algorithm to decompose the stochastic space in orthogonal complement subspaces, through a one-to-one mapping to a non-overlapping domain decomposition of the region of interest. The localization of the search is performed by Gibbs sampling: we apply a KLE expansion locally, at the subdomain level.

The effectiveness of the proposed framework is tested in the solution of inverse problems related to elliptic partial differential equations. We use multi-chain studies in a multi-GPU cluster to show that the new algorithm clearly improves the convergence rate of the preconditioned MCMC method.

**Time Block Preference:**

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## **Multiscale modeling and simulation of microbially-induced calcite precipitation in porous media**

**Author:** Yurong Yang<sup>None</sup>

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Microbially induced calcite precipitation (MICP) in soils can be fundamentally explained by combined theories of reactive transport and metabolic-related biological activities in porous media. Still, it is challenging to describe both the biofilm growth and mineral precipitation at smaller scales, yet their competition and effects on larger-scale transport behaviors remain unclear. To advance the understanding of the MICP process, especially the mechanisms at the pore scale and its effect at larger scales, we hereby present a multiscale porous media model that couples fluid flow, reactive transport and biofilm growth. The coupled model is developed under the Darcy - Brinkman - Stokes equation



(DBS) framework, embedded in OpenFOAM then applied to simulate the MICP in synthetic porous media. Results show that the proposed model can capture the evolving transport processes including urea hydrolysis promoted by microorganisms, the co-play of the biofilm growth and CaCO<sub>3</sub> precipitation, and the fluid flow under the influence of the dynamic change of the pore morphology. A series of impact factors on the MICP process, such as the initial biomass, rates of fluid flow, chemical reaction and biofilm growth, as well as the interplay between biofilm and CaCO<sub>3</sub> precipitation, are also analyzed.

#### Time Block Preference:

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## Multiscale pore network modeling of a carbonate rock sample using micro-CT and SEM images

**Authors:** Gwenole Tallec<sup>None</sup> ; Arsalan Zolfaghari<sup>None</sup>

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Accurate representation of the pore space is of utmost importance in the modeling of flow and transport in porous media. The challenge arises in heterogeneous rocks particularly with wide pore size distributions where the ratio of smaller pores to the sample size is very small. This is obvious, for instance, in the pore-level images of most carbonates where there is a trade-off between resolution and image size. This broad distribution of pore sizes often causes smaller elements, called micro-pores and throats, to be overlooked. However, they can largely affect the flow and electrical properties in porous media.

Modern 3D imaging techniques allow characterizing porous rock samples at different scales, by using computed tomography and electron microscopes.

However, for heterogeneous porous samples such as carbonates, with simple mineralogy but very complex pore space, extracting accurate petrophysical properties and simulating fluid flow is challenging.

Yet global methods, including LBM or PNM simulations, are not predictive unless they take into account the heterogeneity of the pore space by computing local properties at each scale and upscaling them using appropriate algorithms.

The goal of this study is to simulate multiphase flows as accurately as possible for a middle-eastern heterogeneous carbonate rock sample, and to define a workflow for further experiments on similar rocks.

In this study, we will mix classical segmentation of microCT samples with modern image processing routines such as machine and deep learning to automatically segregate the rock structure into the matrix, macroporous, and microporous regions. Machine and Deep Learning have a great interest to be user-independent and automated, hence producing extremely trustable outputs.

Moreover, this workflow is independent of the PC memory since all computations are run out of memory to get rid of the hardware limitation. All operations can be automatized for further replications to other samples.

A 7,5 cm tall and 38mm large plug has been scanned with a high-resolution microCT at a resolution of 16  $\mu\text{m}$ .

The analysis shows that the pore space is not entirely resolved, hence a 10mm diameter sub-plug has been extracted and scanned at a resolution of 5 $\mu\text{m}$ .

The sample being highly heterogeneous with an important micro porous region even not resolved at the resolution of 5 $\mu\text{m}$ , the sub-plug has been cut and scanned with an SEM at a resolution of 2 $\mu\text{m}$ , which was considered enough to resolve the smallest pores.

We have then used a process-based modeling approach to generate 3D representations of the sample from SEM image information. Excluding the macroporous regions, we obtain pore space representations of the microporous regions. This can be repeated for each realization of the process-based modeling. These realizations are then simulated using pore network modeling to obtain the upscaled flow and electrical properties. This process generates different rock types for each of the generated realizations. These rock types are then inputted in the multiscale pore network extraction model to generate hybrid pore network models. These hybrid pore network models are then used to simulate multiphase flow and query the relative permeability of the entire rock sample.

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A Multiscale Imaging and Modeling Workflow for Tight Rocks, Leonardo Ruscpini&Al **Acceptance of Terms and Conditions:**

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## Nano-scale wetting film impact on multiphase transport properties in porous media

**Authors:** wenhui song<sup>1</sup> ; Masa Prodanovic<sup>2</sup> ; Jun Yao<sup>None</sup> ; Kai Zhang<sup>3</sup>

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The multiphase distribution and transport properties in porous media are strongly influenced by capillary pressure and rock-fluid interactions. The influence of nano-scale wetting film caused by the disjoining pressure on the multiphase transport properties is not fully considered in the current pore scale modeling methods and it is unclear how the nano-scale wetting film influences the transport behavior. In this study, we propose a multiphase pore network transport model that considers both capillary pressure and disjoining pressure (the latter arising only in fluid films on solid surfaces). The thickness of nano-scale wetting film under multiphase conditions in irregular pores is calculated based on the force balance between capillary pressure and disjoining pressure resulting from van der Waals force, electric double-layer interactions and structural force. The gas displacing water process is simulated in a water-wet 3D unstructured pore network extracted from 3D reconstructed digitized shale image. The influence of nano-scale wetting film on essential transport parameters including relative permeability, capillary pressure curve and resistivity index is analyzed and its variation is elucidated for different porous media length scale. Notably, the nano-scale wetting film enhances the wetting phase relative permeability and electrical conductivity in nano-scale porous media, and the effect is way less important on micron-scale. Furthermore, we found that the nano-scale wetting film causes more wetting fluid retention after displacement in nanoporous media, which possibly explains the low flowback rate after hydraulic fracturing in shale and ultra-tight sandstones.

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## Nanofluid Evaluation for Enhanced Oil Recovery

**Authors:** DAVID ANTONIO ARGUIJO MUÑIZ<sup>1</sup> ; Ana Paulina Gómora Figueroa<sup>1</sup>

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**Title:** Nanofluid Evaluation for Enhanced Oil Recovery

Nanotechnology has the potential to upgrade the oil and gas industry within different areas such as exploration, drilling, production, and enhanced oil recovery (EOR). For instance, the use of nanoparticles as an EOR method exhibit many advantages since: 1) The size and shape of nanoparticles can be easily modified during fabrication. 2) Nanoparticles' surface chemical properties can be easily adapted to turn them hydrophobic or hydrophilic and modify the chemical interaction with specific types of surfaces. 3) Nanoparticles may resist harder conditions in comparison with conventional EOR chemical methods.

During the last decade, numerous studies have been conducted employing nanoparticles for EOR purposes. Different types of nanoparticles, organic and inorganic, show a significant increase in the recovery of crude oil. These results are encouraging, specifically for mature fields.

In Mexico's case, most of the light and medium crude oil fields are mature and waterflooding for pressure maintenance and have shown promising results at increasing oil recovery. The available infrastructure for waterflooding could be used for nanofluid injection pilot tests; however, it is necessary to generate more data regarding rock properties, multiphase flow behavior, and the interaction among the porous media and the fluids. Also, it is essential to count with experimental data about the efficiency and dynamics of oil recovery acquired by injecting the nanofluid as the "displacing fluid."

Our team recently synthesized LIRF-1 nanoparticle to form Pickering emulsions and study; 1) the effect on the interfacial tension of oil/water mix (mineral and vegetable oils), 2) the displacement of oil in capillary tubes, and 3) the wettability alteration in sandstones by simple imbibition tests.

This work presents the evaluation of LIRF-1 in the formation of Pickering emulsions (O/W) using mineral ( $\rho=0.920$  g/cm<sup>3</sup> and  $\rho=0.84$  g/cm<sup>3</sup>) and Mexican crude (28 °API) oils at different ratios (water to oil), salinity, and nanoparticle concentrations. Also, we carried out oil displacement and core flooding tests, using Berea sandstone to evaluate the interactions between rock-nanoparticles and fluids. Preliminary results showed that nanoparticles displaced up to 50 % of the oil compared to 26 % of oil displaced by brines. Finally, we performed different experiments to measure the contact angle variations and estimate the porous media's wettability alteration by the LIRF-1 nanofluids.

The authors thank funding from PAPIIT IA105621 and CONACYT 280816.

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Time Block C (18:00-21:00 CET) **References:**

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MS25 / 418

## Near-term forecasts of soil water states

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Soil water content (aka soil moisture) influences many Earth surface processes, from surface runoff to ET to groundwater recharge. By combining pedotransfer functions (PTF's) (e.g., Vereecken, 1995; Vereecken et al., 2010; van Looy et al. 2017), digital soil models, and high-resolution weather forecasts, we can estimate future soil water states (content and storage), and then use them to solve practical problems like flood risk potential and irrigation needs. Especially where human wellbeing is concerned, errors in soil water state estimates need to be minimized. The questions we ask are: what is our current skill in forecasting soil water content and storage, and what is the role of soil hydraulic properties in reducing errors in these forecasts? To address these questions, we use data from the Texas Soil Observation Network (TxSON), which monitors soil water states and weather parameters from 40 sites, all located west of Austin, TX. Weather forecasts are available from the US National Weather Service (NWS) at time resolutions that vary between 1-12 hours, depending on forecast period, and initial soil hydraulic properties are obtained from PTF's using SoilGrids250m (Hengl et al., 2017). The monitored field site(s) are found on thin, calcareous soils formed on limestone parent material. Vegetation consists of oak trees, woody plants, and a mixture of short and mid-height grasses (Caldwell et al., 2019). Data are incorporated into HYDRUS-1D, where we fine tune soil properties across several months that includes wet and dry periods. We then forecast soil water states between May 2020 – February 2021, using HYDRUS-1D and 7-day weather forecasts obtained from the NWS's National Blend of Models (NBM). NBM provides highly-skilled weather forecasts, with data including probability of precipitation, temperature, wind speed and direction, dew point, etc. from which forecasts of ET—and soil water states—can be obtained. Forecasts of soil water content are compared sequentially to measurements from ground-based sensors. As simulations move forward in time, each 7 days long, multiple comparisons of observed and forecasted soil water states are determined as forecast lead time is reduced from 7 days to 0 days. Conducted over ~300 days, stacked results will indicate when errors in soil water forecasts drop below a specified threshold (e.g., +/- 0.03 m<sup>3</sup>/m<sup>3</sup>). Results will be presented in the form of ubRMSE and magnitude difference between observed and forecasted soil water content, as a function of forecast lead times.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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MS21 / 317

## **Non-Newtonian flow in macroscopic heterogeneous porous media: from power-law fluids to rheology with change of behavior**

**Author:** laurent talon<sup>1</sup>

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Many natural or industrial fluids exhibit non-Newtonian behavior. Non-Newtonian fluids can therefore be found in different applications related to porous or fractured media such as mud flows, oil recovery, hydraulic fracturing or foam injection clean-up.

Although there are many different non-Newtonian fluids, we focus in this work on fluids that exhibit a change in regime: for low shear-rate, their viscosity is constant (Newtonian) but it becomes shear-thinning (or shear-thickening) at higher shear rate.

And we are interested in understanding the flow of these fluids in large scale heterogeneous porous media, and particularly in the coupling between flow heterogeneity and the rheology.

Since the local viscosity changes above a certain velocity threshold, the flow field depends drastically on the mean flow rate or the applied pressure drop. In particular, one expects that the flow condition affects drastically the velocity field inhomogeneity, which is an important feature to understand the transport of species. We will show that, if the flow presents two asymptotic regimes of low and high flow rate corresponding to power-law fluids, the transition between these two regimes characterizes the heterogeneity of the permeability field. And, similarly to the case of yield stress fluids, the flow field presents interesting geometrical characteristics in this transitional regime, such as criticality and multi-scale (fractal) properties which will be analyzed.

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MS10 / 575

## **Non-destructive 3D mapping of mineral composition and clay mineral orientation in shale**

**Author:** Fredrik K. Mürer<sup>1</sup>

**Co-authors:** Aldritt S. Madathiparambil<sup>1</sup> ; Kim Robert Tekseth<sup>2</sup> ; Pierre Cerasi<sup>3</sup> ; Basab Chattopadhyay<sup>2</sup> ; Dag Werner Breiby<sup>2</sup>

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Shales are sedimentary rocks with a complex mineralogy, where the mechanical properties are predominantly determined by the orientation of clay minerals<sup>1</sup>. Shales are increasingly studied, due to their use as cap rocks in carbon capture and storage (CCS) technologies. Attenuation-contrast computed tomography (CT) allows three-dimensional (3D) imaging of the microscale morphology, also allowing identification of some high-density inclusions. However, attempts at segmenting the attenuation-CT tomograms can be ill-defined or even impossible, as the hierarchical material contains mineralogical features at the nanoscale<sup>[2]</sup>, thus giving partial volume effects precluding reliable assignment of sample compositions to the observed grayscale values. Better methods for 3D non-destructive imaging of shales are therefore in high demand.

X-ray diffraction computed tomography (XRD-CT) is a recent 3D imaging technique relying on synchrotron X-ray diffraction (XRD) as a mineral-sensitive contrast mechanism<sup>[3]</sup>. The chemical composition and mineralogy can be spatially resolved with micrometre resolution, allowing 3D mapping of minerals, which is crucial to image samples where physical sectioning of the samples risks changing the delicate sample microstructure, as is the case for shales. The diffracted X-rays additionally provide information about the crystallite orientation found in the sample, and can be mapped in 3D using X-ray diffraction tensor tomography (XRDTT)<sup>[4–7]</sup>, which is a recent extension of XRD-CT.

Here, we demonstrate the use of XRD-CT to study the mineralogy and clay mineral orientation in Pierre shale. Figure 1a sketches an XRD-CT setup for measurement of a ~3 mm diameter cylindrical sample of Pierre shale. A large number (~10<sup>5</sup>) of diffraction patterns were collected, and these contain information about the mineral composition and crystallite orientation. A corresponding attenuation-contrast CT cross-section is shown in Fig. 1b, revealing that the sample contains several highly attenuating mineral inclusions. The clay minerals are predominantly oriented with their stacking layer normal along the bedding direction (coinciding with the sample cylinder axis, see Fig. 1c). Notably, a band of a slightly different orientation is seen to stretch diagonally across the sample. By using XRDTT analysis, the clay mineral orientation is reconstructed in 3D, and regions of varying clay mineral preferred orientation in the samples are revealed, as shown in Fig. 1d. Additionally, high-density isotropically scattering mineral inclusions were found, and by the XRD analysis, these inclusions could irrevocably be concluded to contain pyrite.

While the voxel size in the current experiment was 50  $\mu\text{m}$ , the continued experimental developments should in the near future allow resolutions below 100 nm. Our results show that XRD-CT/XRDTT is fast becoming a powerful method to study the complex structure of shales.

#### Acknowledgements

We are grateful to the Research Council of Norway for financial funding through FRINATEK (#275182) and its Centres of Excellence funding scheme (#262644).

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MS15 / 503

## Non-intrusive reduced order modeling of natural convection in porous media

**Authors:** Teeratorn Kadeethum<sup>1</sup> ; Francesco Ballarin<sup>2</sup> ; Hongkyu Yoon<sup>3</sup> ; Nikolaos Bouklas<sup>1</sup>

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A simulation tool capable of speeding up the calculation for natural convection in porous media is of sizeable practical interest for engineers, in particular, to effectively perform sensitivity analyses, uncertainty quantification, and optimization of CO<sub>2</sub> sequestration and geothermal harvesting. We present a non-intrusive reduced order model (ROM) using the nested proper orthogonal decomposition (POD) and artificial neural networks (ANN). In this study, the nested POD refers to a compression strategy in which time and uncertain parameter domains are compressed consecutively (in contrast to the classical POD method in which all domains are compressed simultaneously). We utilize the two-field mixed finite element method and interior penalty discontinuous Galerkin approximation for spatial discretization and the 4th-order backward differentiation formula for time-stepping as our full order model (FOM). This combination is selected to avoid spurious oscillations resulting from the lack of local mass conservation and accurately capture the gravity-driven flow in advection-dominated problems. The proposed framework is divided into an offline phase for the ROM construction, which we will present through five consecutive steps and (single-step) online stage for the ROM evaluation. The \textbf{offline phase} includes the following steps: (1) initialize a training set (uncertain parameters), which could correspond to material properties, boundary conditions, or geometric characteristics, (2) query the FOM for each value in the training set, (3) compress the FOM results using the nested POD, (4) obtain the optimal representation of the FOM results employing an  $L^2$  projection, and (5) train the ANN to map the set of uncertain parameters (input) to the collection of coefficients calculated from an  $L^2$  projection over the reduced basis (output). During the \textbf{online phase}, for given values of uncertain parameters, we aim to recover the online approximation of our primary variables by querying the ANN evaluation of the collection of coefficients and reconstructing the resulting finite element representation through the reduced basis functions. We conclude the presentation using a series of validations through the method of manufactured solutions used in and benchmark problems of the Horton–Rogers–Lapwood and Elder problems.

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MS25 / 446

## Non-invasive characterization of soils and aquifers: 20 years of hydrogeophysics at the Agrosphere institute

**Authors:** Johan Alexander Huisman<sup>None</sup> ; Anja Klotzsche<sup>1</sup> ; Jan van der Kruk<sup>1</sup>

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Progress in the fields of vadose zone and groundwater hydrology is still hampered by the challenges associated with the characterization of the multi-scale heterogeneity of the subsurface environment. Hydrogeophysics attempts to address this challenge by providing methods that allow the non-invasive characterization of subsurface structures (e.g., layering, sedimentology) and their interaction with processes (e.g., water flow, solute transport). In this presentation, we will provide an overview of developments in the field of hydrogeophysics in the past two decades using examples from research at the Agrosphere institute under the supervision and guidance of Harry Vereecken. After an introduction of the hydrogeological test site Krauthausen that motivated the initial geophysical endeavors at the Agrosphere institute, we will first review developments with geophysical instrumentation and data interpretation methods, including spectral induced polarization and full-waveform inversion of ground penetrating radar data. After this, the high value of time-lapse geophysical measurements for process investigations will be illustrated. In particular, we will present electrical resistivity tomography measurements used to monitor tracer movement at the Krauthausen test site, and ground penetrating radar measurements in horizontal boreholes used to monitor water content dynamics in the vadose zone of a rhizotron facility operated in Jülich. These two case studies will also be used to discuss strategies to integrate geophysical measurements and hydrological models. Due to the high mobility of some geophysical sensors, hydrogeophysical research is increasingly moving towards investigations beyond the field scale. This will be illustrated using a study where electromagnetic induction measurements were used to derive a geophysics-based soil map that can be used to support within-field management in the context of sustainable crop production. Taken together, the presented case studies will highlight the developments in the field of hydrogeophysics and the remaining challenges that will need to be addressed in future studies.

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MS19 / 565

## Non-solvent Induced Phase Separation: A Synthetic Approach Towards High Performance Redox Flow Battery Electrodes

**Author:** Rémy Richard Jacquemond<sup>1</sup>

**Co-authors:** Charles Tai-Chieh Wan<sup>2</sup> ; Yet-Ming Chiang<sup>3</sup> ; Kitty Nijmeijer<sup>4</sup> ; Fikile R. Brushett<sup>5</sup> ; Antoni Forner-Cuenca<sup>6</sup>

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**Corresponding Authors:** d.c.nijmeijer@tue.nl, brushett@mit.edu, r.r.jacquemond@tue.nl, a.fornier.cuenca@tue.nl, ychiang@mit.edu, ctwan@mit.edu

Transitioning to a sustainable energy economy is one of the greatest challenges of this century. Integrating renewables (e.g., wind and solar power) into the grid must be accelerated to limit the devastating effects of climate change. Due to their intrinsic intermittency, large-scale energy storage must be deployed to balance the mismatch between supply and demand<sup>1</sup>. Redox flow batteries (RFBs) stand out as a promising candidate due to their ability to independently scale power and energy and projected lower costs<sup>[2,3]</sup>. The performance of RFBs largely depends on the porous electrodes microstructure and chemical composition as they must simultaneously provide high surface area for electrochemical reactions, low pressure drop, high electrical conductivity, and facile mass transport<sup>[4]</sup>. State-of-the-art electrodes are composed of carbon fibers which are arranged together using mechanical methods forming idiosyncratic structures such as papers, cloths and felts<sup>[5]</sup>. Their fabrication involves multiple complex subprocessing steps<sup>[6]</sup> impacting the final manufacturing cost and offering limited versatility to control the three-dimensional structure of the material, which ultimately hampers widespread commercialization of the technology.

Here, we introduce the non-solvent induced phase separation (NIPS) as a simple and versatile fabrication method for carbonaceous porous electrodes<sup>[7]</sup>. Drawing inspiration from membrane science and technology<sup>[8]</sup>, the NIPS method has been leveraged to synthesize morphologically-diverse microstructures (e.g., isoporous, macrovoids, porosity gradient) which are appealing to electrode manufacturing. A polymer solution, containing polyacrylonitrile (PAN, carbon-containing) and polyvinylpyrrolidone (PVP, pore-forming agent) dissolved in N,N-dimethylformamide (solvent) was casted in a mold and subsequently immersed in water (non-solvent). Finally, the polymeric scaffold is carbonized under inert conditions to form a conductive network. Easily adjustable parameters, such as solvent type, polymer concentration and temperature enable control of the final electrode microstructure. In this work, we study the influence of the PAN:PVP ratio on the electrode microstructure and its resulting effect on RFBs performance.

Microstructural characterization revealed a multimodal pore size distribution composed of fine, interconnected microvoids (pore diameter  $\approx$  2-15 $\mu$ m) coupled with through plane, finger-like macrovoid channels (throat diameter > 50  $\mu$ m) forming honeycomb networks. The unique microstructure, not attainable with traditional carbon-fiber manufacturing techniques, enables large surface area at the membrane-electrode interface and fast electrolyte replenishing which reduces mass transfer resistance within the electrode. Flow battery tests with Fe<sup>2+</sup>/Fe<sup>3+</sup> electrolyte revealed a considerable reduction of the charge transfer (RCT  $\approx$  0.016  $\Omega$ ) and mass transfer (RMT  $\approx$  0.025  $\Omega$ ) overpotentials of the novel electrodes compared to the commercial baseline (SGL29AA, RCT  $\approx$  0.326  $\Omega$  and RMT  $\approx$  0.151  $\Omega$  at a linear velocity of 5 cm s<sup>-1</sup>) at the expense of a slight increase in pressure drop. In the final part, we demonstrate the use of NIPS-electrodes in a full all-vanadium RFB. The polarization analysis revealed a ca. 70% improvement in power density compared to the baseline material, which can be attributed to reductions in the charge transfer and mass transport overpotentials. Although nascent, NIPS emerges as a promising platform to engineer porous electrodes for RFBs and other convection-enhanced electrochemical systems.

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MS6-A / 22

## Non-thermal Fluctuations in Stead-State Multiphase Flow in Porous Media

**Authors:** Maja Ruecker<sup>1</sup> ; Steffen Berg<sup>2</sup> ; Apostolos Georgiadis<sup>2</sup> ; Ryan Armstrong<sup>None</sup> ; Holger Ott<sup>3</sup> ; Niels Brussee<sup>2</sup> ; Hilbert van der Linde<sup>4</sup> ; Frieder Enzmann<sup>None</sup> ; Michael Kersten<sup>5</sup>

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Relative permeability is typically measured in core flooding experiments where the so-called steady-state method is preferred over other approaches because of the large accessible saturation range, better control and interpretability compared with other methods. Wetting and non-wetting phases are co-injected at a range of fractional flows  $f_w$  and the resulting pressure drop and saturation are monitored. These experiments are typically performed on cylindrical samples of preferentially homogeneous porous media (e.g. rock) of several centimeters in length and diameter. The implicit assumption is that these samples are sufficiently large to represent Darcy scale flow which is supported by the fact that e.g. in homogeneous sandstone rock the porosity and permeability representative elementary volume (REV) is just 3-4 mm. The common understanding of Darcy-scale flow regimes is that pore scale phenomena and their signature should have averaged out at the scale of representative elementary volumes (REV) and above. However, many steady-state relative permeability experiments exhibit temporal variations in key parameters such as pressure drop and saturation. In the past these fluctuations have been largely mistaken for experimental artefacts caused by e.g. membrane-based back pressure regulators. However, a number of experiments where such instrument-based artefacts can be ruled out suggest that there is an intrinsic cause of these fluctuations related to the underlying pore scale flow regimes.

By comparing the signature of the fluctuations between a centimeter scale experiment with in-situ saturation monitoring and a pore scale experiments with 3D imaging by synchrotron beamline-based fast X-ray computed micro tomography we establish that large fluctuations which are associated with a capillary energy scale (many orders of magnitude larger than thermal fluctuations) are much larger than instrumental noise. Instead, they are caused by cascades of pore scale displacement events involving hundreds to thousands of pores. The fluctuations exhibit non-Gaussian statistics and are in some cases repetitive and even oscillatory manifesting themselves in repetitive sequences of travelling saturation waves. Their origin can be traced back to the non-wetting phase cluster ganglion dynamics at pore scale which involve breakup and coalescence processes depending on the fractional flow. Breakup and coalescence processes follow "trajectories" in a "phase diagram" defined by fractional flow and capillary number which can be used to categorize flow regimes. Connected pathway flow would be represented by a fixed point.

Ganglion dynamics occurred even at very small capillary numbers i.e. in a by macroscopic definition clearly capillary-dominated regime which suggests that breakup and coalescence processes are not caused by viscous mobilization. Instead, displacement processes associated with the fractional flow conditions trigger capillary instabilities in a largely metastable pore scale fluid configuration which initiate avalanche-like cascades of displacement events involving a significant number of pores which can lead to not only notable pressure but also saturation changes at the centimeter scale.

Since the steady-state experiment is primarily a stationary state (rather than a steady-state) these fluctuations do average out when applying sufficiently time averages.

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MS17 / 134

## Numerical Modeling for the Reactive Process of Thermochemical Energy Storage Based on Lattice Boltzmann Method

**Authors:** Bin Guo<sup>1</sup> ; Huijin Xu<sup>1</sup>

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The energy storage technology is capable to fill the gap between energy demand and supply and make the renewable energy more efficient, which have also become the research emphasis recently. Among three existing energy storage techniques, thermochemical energy storage has the highest energy density and longest storage period. In this study, we constructed a two-dimensional numerical model of a CaO/Ca(OH)<sub>2</sub> thermochemical energy storage reactor, using lattice Boltzmann method to calculate the whole process. This method is efficient and able to deal with complex boundaries. With regard to CaO/Ca(OH)<sub>2</sub> energy storage process, it is based on the reaction of CaO with water vapor, which can be considered as heterogeneous gas-solid reaction. According to previous relevant researches, the model in this study consists of two parts, fluid area and solid area. The fluid (H<sub>2</sub>O) flows in from one side and out the other, which interacts with the solid particles (CaO), which is similar to previous model. A few reasonable assumptions were taken: the diffusion of fluid in solid phase was ignored; the gas-solid interface followed the first-order kinetics model; the heterogeneous reactions only happened at the interface. Besides, the solid update algorithm was adopted in order to describe the phenomenon that the mass and volume of solid changes during the reaction, which means the flow state also changes as the reaction goes. When the result reached steady state, the reaction stopped. Additionally, the heat emitted by the reaction was determined by the reaction condition of each solid node, so this study is composed of flow, mass and heat transfer problems. It can help researchers to learn about more mechanisms of CaO/Ca(OH)<sub>2</sub> energy storage and find out better solutions of promoting the efficiency of thermochemical storage reactor, which has great significances.

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MS19 / 91

## Numerical Modeling of Capillary-Driven, Paper-Based, Flow-Through, Microfluidic Redox Flow-Batteries

**Authors:** Pardis Sadeghi<sup>1</sup> ; Erik Kjeang<sup>1</sup>

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During the last couple of decades, interest in small-sized, single-use, disposable devices such as rapid diagnostic kits (RDK's) has dramatically soared [1]. Currently, such portable electronic devices rely heavily on conventional coin/button cell batteries for their operation. Although such batteries are very reliable and efficient, they become troublesome when such single-use kits have to be disposed of. The problem is that the kits are usually discarded when the battery is not fully discharged. Evidently, this means a huge waste of energy, but, more importantly, it poses severe environmental hazards when the chemicals stored inside the battery diffuse into aquifers. In a world re-imagined with bio-degradable materials, it is of no surprise that in recent years we are witnessing a growing interest in cellulosic materials for the construction of such kits. Paper is cheap, recyclable, and bio-degradable. An extra feature of cellulosic paper is that they can be used in the context of a flow battery to energize the printed circuitry of such kits [2]. That is to say that, while test fluid such as urine or blood is laterally spreading through the paper, they can serve as the fuel to energize the kit. As a matter of fact, the electrodes can be as simple as two parallel lines sketched by just a pencil on the two edges of the cellulosic paper. Fortunately, in recent years, novel paper-based, all-quinone, flow-through, microfluidic flow batteries such as PowerPAD have been developed for single-use applications [3]. The cellulosic absorbent pad incorporated in the design of this flow battery establishes flow through its porous carbon electrodes via capillary action thereby eliminating the need for any type of micropump. The device is inherently transient as it relies on passive, dynamic wicking of electrolytes through the porous electrodes where electrochemical reactions occur. But, the power output of this promising flow battery should further be enhanced before it can be considered as a true contender to conventional batteries. And this requires that a mathematical model is available which can be used for its design. In this work, a general theoretical framework has been developed for designing such flow batteries. The proposed two-step methodology can be used for determining the polarization curves of such electrochemical cells at discrete times. Results obtained this way can then be used to investigate the effect of different parameters on the maximum power output of the cell and its efficiency as functions of time. In our two-step methodology, imbibition of electrolytes by electrode/pad is computed first using Richards equation combined with the Brooks-Corey correlations. In the second stage, the saturation field so obtained is used to obtain the time-dependent velocity field from which polarization curves can be obtained at discrete times. Using a two-dimensional finite-element analysis, we have been able to qualitatively predict the time-dependent behavior of the PowerPAD battery [3]. The methodology developed in this work has also enabled us to qualitatively investigate the effect of pad's thickness, pore size, pore-size distribution, and contact angle on the power output of this battery.

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## **Numerical Simulation of CO<sub>2</sub> Huff-n-Puff to Enhance Oil Recovery from Tight Oil Reservoirs. A Case Study.**

**Author:** Ayman Mutahar AlRassas<sup>1</sup>

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The integration of horizontal well drilling and hydraulic fracturing has improved oil production from tight oil reservoirs. The oil recovery potential using primary recovery is cumbersome due to its robust tight formation; thus, the remaining oil in place in the tight oil reservoir required an effective method to improve the oil recovery from the tight oil reservoir. The implementation of CO<sub>2</sub>-EOR has substantiated its ability to boost oil recovery from tight oil reservoirs. In this study, a numerical simulation of CO<sub>2</sub> injection huff & Puff was conducted—three series of CO<sub>2</sub> injection, CO<sub>2</sub> shut-in, and production. Huff&Puff is effective to compare to CO<sub>2</sub> flood, as CO<sub>2</sub> flooding required a long time for pressure dissipation from the injection and production well. Reservoir heterogeneity, permeability, fracture half-length, number of cycles, and the effectiveness of CO<sub>2</sub> on the efficiency of huff& Puff were investigated. The result indicates that CO<sub>2</sub> propagation in the tight oil reservoir plays a substantial role in enhancing oil recovery from the tight oil reservoirs, emphasizing that CO<sub>2</sub> in heterogeneity, low-permeability, and extend fracture half-length is more preferable as it was aforementioned. This paper elucidates the performance of CO<sub>2</sub> Huff&Puff in the tight oil reservoir of the Bakken formation, North America.

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MS3 / 651

## Numerical Simulation of Coupling Darcy and Forchheimer Flow in the Carbonate Reservoir

**Authors:** Yueying Wang<sup>None</sup> ; Sebastian Geiger<sup>None</sup> ; Jun Yao<sup>None</sup>

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The carbonate reservoir is one of the important reservoir types, while they are different from the conventional reservoirs. They are very complex and are characterized by serious heterogeneity and multi-scales, the porosity scale is from the millimeter level to the meter level, thus there is not only the Darcy flow but also nonDarcy flow in the subsurface. It means it is hard to simulate the fluid flow in them only using the Darcy equation or Forchheimer equation. It is necessary for the researcher to develop a linkage model which can be used for the coexistence of the Darcy stream and the Forchheimer stream. We develop the coupling model in which the Darcy flow and Forchheimer flow are all considered. The Darcy equation and the Forchheimer equation are different and they have the different ranges of applicability. To integrate simultaneously Darcy flow and Forchheimer flow, they should satisfy the boundary condition on the interface of the boundaries: the pressures should be equal, and the fluid flow should be conservative. We built the governing equation of coupling model through the coupling boundary conditions, and the numerical simulation is realized by using Control-volume method. It has been verified the validity and correctness of the coupling boundary condition from two aspects: theory and numerical solution. The numerical simulation results prove not only the correctness and feasibility of the coupling model, but also the advantage of the coupling model in the carbonate reservoir.

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MS25 / 448

## Numerical modeling to optimize nitrogen fertigation with consideration of transient drought and nitrogen stress

**Author:** Thomas Groenveld<sup>1</sup>

**Co-authors:** Amir Argaman<sup>1</sup>; Jiří Šimůnek<sup>2</sup>; Naftali Lazarovitch<sup>1</sup>

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Optimization of nitrogen (N) fertigation is a formidable challenge involving complex interactions between water and N uptake and their effects on crop production. Numerical models can be useful in studying the interaction of multiple variables like those found in mechanistic simulations of N fertigation strategies. The physical aspects can often be accurately represented in soil-plant-atmosphere continuum models, while the biological factors lag due to their oversimplification. When optimizing N fertigation using numerical models, it is essential to consider the effects of N and water stresses on the plant size and corresponding feedback on potential transpiration and N uptake.

The HYDRUS (2D/3D) model was modified to allow for active uptake and decay of multiple solutes and reduce potential transpiration due to a limitation in N uptake. Subsequently, we calibrated and validated the model with a dataset that consisted of 3 nitrate (NO<sub>3</sub><sup>-</sup>) concentration and 6 irrigation levels: a total of 18 distinct treatments used to fertigate cucumber plants grown in lysimeters. The calibration was based on the treatment that received the highest N fertigation. The model was validated by testing its ability to accurately reduce potential N uptake and transpiration in water and N deficiency cases.

Simulations showed that the N stress function could explain 82% of the reduction in transpiration measured in the experimental setup. The sensitivity analysis, evaluating the effects of the root shape and distribution parameters by increasing and decreasing their values by 20%, showed that these parameters had little impact on the results. Following its validation, the model was used to determine the optimal N concentration in irrigation water and the optimal N application amount to obtain maximal yield with minimal N loss. The optimal irrigation water NO<sub>3</sub>-N concentration and seasonal NO<sub>3</sub>-N application were determined to be 75 mg L<sup>-1</sup> and 40 mg m<sup>-2</sup>, respectively.

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MS20 / 676

## Numerical modelling and experimental validation of percutaneous vertebroplasty

**Author:** Zubin Trivedi<sup>None</sup>

**Co-authors:** Dominic Gehweiler ; Christian Bleiler ; Arndt Wagner ; Tim Ricken<sup>1</sup> ; Boyko Gueorguiev-Rüegg ; Oliver Röhrle

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Percutaneous vertebroplasty is a medical procedure done for treating weakened or damaged vertebrae. In this procedure, a cement-like polymer (bone cement) is injected percutaneously into the inside of the vertebra, which is a porous trabecular structure. Upon curing, the bone cement restores the structural strength of the vertebra. While the procedure is fairly successful, there is a risk of bone-cement leaking outside the vertebra, which could lead to severe problems like pulmonary embolism or paralysis. Towards this, a numerical model that can simulate the flow of bone cement inside the porous vertebra could be useful. Such a model could help mitigate the risk of leakage and help the surgeons determine optimum operating parameters, viz. the injection pressure, the cement viscosity, etc.

However, the problem is particularly challenging due to many factors like the complex geometry of the trabecular structure, the curing of the bone cement, non-Newtonian rheology of the bone cement and the bone marrow, and patient-to-patient variation in material parameters. In order to tackle this, a continuum-mechanical approach based on the Theory of Porous Media is used to develop a multiphase model consisting of bone, bone marrow, and bone cement. The flow is modelled using a fully upwind Galerkin formulation. Rheological modelling of the fluids is done using non-Newtonian (shear-thinning) constitutive equations. The viscosity at the macro-scale is obtained using semi-empirical models to upscale the shear-rate. The curing of bone cement is modelled by adding a time-dependence to its viscosity. Rheological characterisation of the bone cement is carried out to obtain the material parameters. For the validation of the model, an experiment is set up where the bone cement is injected into representative porous media (here, aluminium foam). The evolution of the flow is captured using a dynamic CT imaging setup. The results at the different stages of injection are then compared and studied.

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MS1 / 229

## Numerical modelling workflow for the assessment of long term CO<sub>2</sub> storage in saline aquifers using the Sleipner dataset

**Author:** Takashi Akai<sup>1</sup>

**Co-authors:** Daima Hasegawa<sup>2</sup>; Hiroshi Okabe<sup>1</sup>

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CO<sub>2</sub> injection in deep saline aquifer formations is a promising scheme to reduce the emissions of CO<sub>2</sub> into the atmosphere. The migration of injected CO<sub>2</sub> can be characterized as multiphase flow in porous media where CO<sub>2</sub> displaces brine in porous reservoir rocks. The migration observed with 4D seismic data often suggests that the shape of a CO<sub>2</sub> plume is strongly affected by thin shale layers interbedded within a target reservoir formation – impermeable shale layers often act as a flow barrier against the upward migration of CO<sub>2</sub>. To capture this migration behaviour, it is necessary to use an extremely high-resolution grid system that explicitly models thin shale layers whose thickness can be less than 1m.

Reservoir simulation software based on Darcy's law is commonly used to study the migration of CO<sub>2</sub> at the field scale. However, the use of the Darcy simulator with a fine resolution model takes an extremely long computation time. Another approach to simulate multiphase flow in porous media is to use the invasion percolation theory (IP). This IP simulator determines percolation pathways based

on the Young-Laplace relationship. Thanks to the simplification of the physics, an IP simulator is more computationally efficient than a Darcy simulator.

We show a numerical modelling workflow that uses both IP and Darcy simulator using the data obtained in the Sleipner CCS project<sup>1</sup>. First, we used an IP simulator to match the shape of the simulated CO<sub>2</sub> plume with that observed with 4D seismic data. The use of an IP simulator made it possible to explore a wide range of parameter space of reservoir properties with an extremely fine grid system that can explicitly capture thin shale layers in the reservoir. As a result, the simulated CO<sub>2</sub> plume distribution showed a good agreement with that obtained with the 4D seismic data. Furthermore, this history matched model was then converted to a Darcy simulator to incorporate additional physics which plays an important role in long term CO<sub>2</sub> storage (e.g., the dissolution of CO<sub>2</sub> in brine and the diffusion of CO<sub>2</sub> in both gas and brine). Using this Darcy model, we performed long-term CO<sub>2</sub> storage simulations for more than 1000 years to investigate the change in the CO<sub>2</sub> storage mechanism over time.

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MS24 / 299

## Numerical scheme for a coupled system in geomechanics

**Authors:** Adrien Beguin<sup>1</sup> ; Danielle Hilhorst<sup>2</sup> ; Ludovic Goudenège<sup>3</sup>

<sup>1</sup> *Paris-Saclay*

<sup>2</sup> *CNRS and University Paris-Saclay*

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Building on the work of Andro Mikelic and Mary Wheeler, we propose a numerical scheme for an elliptic-parabolic system involving deformation and pressure in porous media. Existence and uniqueness of the solution have been proved by Mikelic et al; we will add some convergence results for our numerical scheme.

This is joint work with Ludovic Goudenège and Danielle Hilhorst

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Convergence of iterative coupling for coupled flow and geomechanics, Andro Mikelic and Mary F. Wheeler **Acceptance of Terms and Conditions:**

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## Numerical simulation aiding the development of superhot geothermal resources



**Author:** Thomas Driesner<sup>1</sup>

<sup>1</sup> *ETH Zuerich*

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There is mounting evidence that many conventional high-enthalpy geothermal resources that are exploited for power generation in volcanic areas are underlain by so-called superhot resources. Superhot resources are loosely defined as having a temperature higher than the critical temperature of water (374°C) and enthalpies ideally high enough to not intersect the two-phase region upon production, i.e., can be produced to generate dry, superheated steam. Two wells of the Iceland Deep Drilling project indeed tapped such resources: 450°C at 150 bar in well IDDP-1 at Krafla; and potentially up to >500°C in well IDDP-2 at Reykjanes. Although both cases encountered technical problems that prevented production from the wells, the potential of superhot resources is enormous with possibly up to 10 times more power per well. In order to better understand the geologic controls on and the nature of the resources, numerical simulations turned out to be the tool of choice. A key factor is the effect of the brittle to ductile transition temperature on rock permeability as it controls the maximum temperature of exploitable fluid. In the case of saline fluids, complex phase relations impose that economically attractive reservoirs are more likely to occur above deeper (5 vs. 2-3 km) magmatic intrusions. Furthermore, the salinity of the fluid may determine if and how a well can be started to become self-flowing. The presentation will illustrate key examples to highlight important factors as well as the requirements for meaningful numerical simulations.

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## **Numerical simulation of EGS thermal recovery in Multi-stage Hydraulic Fractured Horizontal Wells**

**Authors:** Guohan Xu<sup>1</sup> ; Hongjun Yin<sup>1</sup> ; Jing Fu<sup>2</sup>

<sup>1</sup> *Department of Petroleum Engineering, Northeast Petroleum University, Daqing 163000, P. R. China*

<sup>2</sup> *Colorado School of Mines, Golden, Colorado, 80401, USA*

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Enhanced Geothermal Systems (EGS) is an effective way to develop deep geothermal energy at high temperature, in order to improve the thermal recovery efficiency of EGS, the multi-stage hydraulic fractured horizontal well technology can effectively transform the reservoir, making the fracture generated by hydraulic fracturing the main heat transfer channel and improving the heat transfer efficiency. Based on the heterogeneity of the reservoir, this paper established the EGS thermal recovery model of multi-stage hydraulic fractured horizontal well. The finite difference method was used to solve the model. The temperature field in the transformed reservoir at different times was obtained, the water breakthrough time of each fracture was calculated, and the parameter sensitivity analysis was carried out. The research results show that the established EGS thermal recovery model can better reflect the heat conduction characteristics of the matrix and the fluid in the fracture, the matrix thermal conductivity coefficient, fracture width, length, number of fractures, thermal recovery time, all have different effects on the temperature field. This study can provide scientific basis for EGS thermal recovery modeling of staged fractured horizontal Wells, and has reference significance for EGS development.

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## Numerical simulation of slope failure in a gas hydrate-bearing continental slope

**Authors:** Sulav Dhakal<sup>1</sup> ; Ipsita Gupta<sup>1</sup>

<sup>1</sup> Louisiana State University

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Gas hydrates are ubiquitous in seabed and submarine rocks in continental slopes around the world. Formation and dissociation of hydrates in porous spaces can alter the geomechanical strength of hydrate-bearing rocks. Dissociation of hydrates in submarine slopes decreases the elastic moduli and cohesion of rocks and can trigger slope failure. Failure of submarine slopes can cause damage to seafloor infrastructures, cause tsunamis, and release methane gas into the atmosphere. The bottom of hydrate-bearing rocks that are indicated by bottom-simulating reflector (BSR) plane can act as the glide plane for failure when large quantities of hydrate dissociate. Based on field observations from Cascadia Margin, a simple two-dimensional bench model is created in FLAC3D, and natural tectonic stress regime is applied. Dissociation of gas hydrate is simulated by a steady depressurization of hydrate-bearing sediments and moduli of elasticity and cohesion are updated based on saturation of gas hydrate. Mohr-Coulomb failure criterion is applied on the poro-elastic model to calculate the factor of safety and failure slope as hydrate saturation decreases. Results from the numerical simulation indicate that the failure slope coincides with the bottom of the hydrate-bearing rock layer. Factor of safety is the ratio between internal frictional angle of the rock to the angle of the slope failure plane relative to the horizon. The factor of safety decreases as hydrate saturation decreases in the hydrate-bearing rock layer. A factor of safety lesser than 1.0 to 1.15 indicates a high probability of slope failure. Results of this numerical simulation is used for validation and verification of field observations, and visualization of slope failure due to hydrate dissociation in continental slopes.

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## Numerical studies of capillary flow in paper-based microfluidic devices

**Author:** Yang Wang<sup>None</sup>

**Co-authors:** Dingding Ye ; Xun Zhu ; Yang Yang ; Chaozhong Qin ; Rong Chen ; Qiang Liao

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Paper-based microfluidic devices are rapidly becoming popular as a platform for developing point-of-care medical diagnostic tests<sup>1</sup>. Capillary force is the main driving force for the transportation of test liquids in paper-based devices. Therefore, a deep understanding of its internal capillary flow are indispensable for designing sensitive and accurate paper-based point-of-care medical diagnostic device. Spontaneous absorption in papers is an unsaturated flow process, which was often modelled by the Richards equation[1-5]. It is well known that two constitutive relationships including relative permeability and capillary pressure are crucial to the model prediction. In this work, we use  $\mu$ CT scanning to obtain the three-dimensional porous structure of a filter paper. The PoreSpy based on the watershed algorithm is used to extract the pore network[6]. A quasi-static pore-network model (QPNM) is used to obtain the capillary pressure and relative permeability relationships. Moreover, we verify the numerical results against lab experiments. Combining imaging technique and pore-network simulations could help us understand material properties of capillary flow in paper-based microfluidic devices, which will guide us to design high-performance paper-based devices.

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MS8 / 658

## Numerical study of dispersion through displacing phase in unsaturated porous media

**Author:** Rasoul Soufi<sup>1</sup>

**Co-authors:** Amir Raof<sup>1</sup> ; Seyed Hossein Mansouri<sup>2</sup>

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Dispersion through unsaturated porous media plays an important role in several industrial and natural processes including those relevant to environmental and hydrogeological applications and chemical and petroleum engineering processes. During recent years, several direct numerical simulations at the pore scale explored dispersion and solute transport in immiscible two-phase flow in porous media. Displacement patterns differ significantly depending on capillary number and viscosity ratios. Different invasion conditions impose important changes on the dispersion of the displacing fluid. Most of studies have not considered the effect of displacement patterns on dispersion through the displacing phase.

This study aims to understand and quantify dispersion in three distinct regimes of displacement including frontal displacement, capillary fingering, and viscous fingering. Hydrodynamic dispersion in all these regimes is modelled in the displacing phase using a volume of fluid (VOF) method in OpenFOAM and compared to a base case to categorize dispersion under different two phase flow regimes. Structure of velocity field and solute transport within the displacing fluid were investigated

to compare dispersion phenomena for each domain. The shape of displacement in each regime causes changes and deviations in dispersion related parameters.

Hydrodynamic dispersion is separated and studied in two parts in our work: with and without diffusion. In the first part the effect of diffusion is investigated, and in the second part statistical parameters of the whole domain and Lagrangian parameters through the domain are explored. Results demonstrate that dispersion of a solute in frontal displacement behaves similar to the base case (i.e., a saturated media) with the same arrangement. Dispersion in the fingering regime is considerably different compared to the base case which can have a significant impact on dispersive behavior of solutes in porous media.

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MS5 / 194

## Numerical study of the temperature effects on MICP

**Author:** Xuerui Wang<sup>1</sup>

**Co-author:** Udo Nackenhorst<sup>2</sup>

<sup>1</sup> *Institute of numerical mechanics and computational mechanics, Leibniz University Hannover*

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Microbially induced calcite precipitation (MICP) is believed to have a great potential to provide eco-friendly solutions to a wide range of geotechnical problems, e.g. mediation of contaminations, improvement of soft underground, erosion control and so forth. Recently, plenty of experimental and numerical investigations have been conducted by many researchers to get a better insight into the processes involved in MICP. Among the current MICP research, especially in the modelling perspective, less attention was paid to the temperature effects. In general, the temperature can affect on the one hand, the chemical reaction rate and on the other hand, the bacterial activities [1-4]. Considering that in the MICP field application, the soil temperature varies along with the underground's depth and changes due to the groundwater flow, thus except for the bio-chemo-hydro-mechanical (BCHM) processes there is still a need to investigate the temperature influence (T).

In the present study a coupled numerical model is developed with the main purpose to investigate the relevant coupled processes, specifically the temperature influence on the microbially induced calcite precipitation (MICP) in soil. The model development is based on the continuum approach in porous media, where the porous media is assumed to be fully saturated. The hydrolysis of urea, the calcite precipitation, bacterial decay and attachment, the transport of bacteria, urea, calcium, and ammonium in the pore fluid, the porosity and permeability reduction are considered. Specifically, to address the temperature influence, the hydrolysis rate of urea is assumed to increase linearly with the temperature elevation. Meanwhile, the inactivation of urease capacity of bacteria with the increased temperature is considered by using an Arrhenius-Type relation. The model is implemented in the open-source finite-element simulator OpenGeoSys (OGS). The spatial discretization is done using the standard Galerkin-Method, while the fully implicit backward Euler-Method is applied for the temporal discretization.

To calibrate, validate, and demonstrate the model's capability, we apply this model to simulate a set of laboratory experiments. The numerical results indicate that the temperature could significantly impact the efficiency and the spatial homogeneity of the calcite precipitation. Thus, as stated in [4], in the application one could improve the performance of MICP by control of the treatment temperature. The numerical simulation could be adopted as a useful tool for the design of such temperature-controlled MICP treatment.

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MS12 / 433

## Numerical yield surface determination of cemented rocks from digital microstructures

**Authors:** Martin Lesueur<sup>1</sup> ; Hadrien Rattiez<sup>2</sup> ; Manolis Veveakis<sup>3</sup>

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Cemented granular materials is a general class of geomaterials composed of grains connected by cement partially or completely filling the void in-between the grains. After deposition and consolidation phases of the sediments, cementation happens during diagenesis when mineral matter precipitates at the pore-grain interface. This process is known to increase the strength of the geomaterial by creating a cohesion between the particles. As such, it is critical to characterize for material stability applications in geotechnical engineering and geophysical processes. However, no quantitative law can be directly derived between the amount of cement and rock strength because cementation depends heavily on the rock microstructure and the initial distribution of chain forces. On top of that, this process takes place at a geological timescale, which makes it complicated to reproduce experimentally. Eventually, only direct numerical simulation of elasto-plasticity performed at the micro-scale level and coupled with microstructure evolution can be used to determine the strength of cemented materials. In this study we provide for the first time a comprehensive parametric study on the impact of cementation on rock strength for real microstructures of granular materials. Compared to most previous studies, the whole yield surface is determined numerically in order to assess the influence of cementation for different stress-paths. The previously known tendency of rock to strengthen with increasing cementation volume is verified. New results on the influence of cement property namely Young's modulus, friction and cohesion on the rock's yield surface are explored. While most studies use Discrete Element Modelling to consider grain contacts explicitly, our simulator uses Finite Element Modelling which allows more flexibility in the approach to model the precipitation of the pressure-sensitive layer of cement. The contacts are modelled as an upscaled plastic law. The framework presented in this study showcases the possibility of determining rock yield surfaces from their microstructures. While the current contribution focuses on cementation, other phenomena of interest can also be investigated such as dissolution from reactive transport.

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## OPTIMUM SEGMENTATION OF A SANDSTONE RESERVOIR MICRO-CT IMAGERY USING MACHINE LEARNING ALGORITHMS

**Author:** Xue Yu<sup>1</sup>

**Co-authors:** Lingyun Kong<sup>2</sup>; Blaise Mibeck<sup>2</sup>; Cesar Barajas-Olalde<sup>3</sup>; Matthew Burton-Kelly<sup>2</sup>; Bethany Kurz<sup>2</sup>; Shane Butler<sup>2</sup>

<sup>1</sup> *National Energy Technology Laboratory; Energy & Environmental Research Center*

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Image analysis of micro-CT (computed tomography) images, which can provide nondestructive evaluation of rock properties (porosity, permeability, etc.), is largely dependent upon optimum segmentation of the image objects. Traditionally, images are segmented using pixel threshold values derived from statistical analysis (e.g., Otsu thresholding method). However, the statistical threshold segmentation algorithms have several constraints that can limit their application: 1) statistical methods return different thresholds that do not converge on a single ground truth; 2) it is difficult to categorize boundary areas where the pixels could belong to several adjacent objects; 3) the contextual relationships of the image objects cannot be included; and 4) domain knowledge of the petrology is required. In this study, we show that supervised machine learning assisted segmentation algorithms can be leveraged to address these issues. In this study, various machine learning algorithms were used to segment the micro-CT images scanned from conventional sandstone reservoir core samples. For supervised machine learning, the labeled images were manually annotated (grain matrix and pores). A traditional machine learning algorithm (random forest classification) and a deep learning algorithm (u-net convolutional neural network) were used in tandem. For the random forest classification algorithm, the feature data set was created by applying various filters to the pixel matrix, such as an image texture capture filter (Gabor filter), edge detection filters (Canny, Roberts, Sobel, Schar, Prewitt), and noise removal filters (Gaussian blurring, median filters). The u-net convolutional neural network is a deep learning algorithm, and it is trained on augmented images to reduce the labor of image annotation. Finally, the performance of the three types of segmentations, i.e., Otsu thresholding, random forest classification and u-net were compared. An optimized segmentation process with higher accuracy and faster speed is essential for further evaluation of pore sizes and 3D microstructures within the sandstone samples at various scales.

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MS9 / 248

## **Oil Displacement by Water Through an Ultra-Narrow Kerogen Pore Throat: a Molecular Dynamic Study**

**Authors:** Yinuo Zhao<sup>1</sup>; Wenhui Li<sup>1</sup>; shiyuan Zhan<sup>2</sup>; Zhehui Jin<sup>1</sup>

<sup>1</sup> *University of Alberta*

<sup>2</sup> *China University of Petroleum (East China)*

**Corresponding Authors:** yinuo8@ualberta.ca, zhanshiyuan321@163.com, zhehui2@ualberta.ca, wenhui4@ualberta.ca

Due to the continuous depletion of conventional oil reservoirs, as an unconventional reservoir, shale plays an increasingly important role to meet the ever-growing global energy demand. Thanks to the extensive number of nano-scale pores and ultra-narrow pore throats (sub-2 nm), shale media is typically subject to an ultra-low permeability. The presence of ultra-narrow pore throats in shale media can greatly reduce oil displacement by water during waterflooding. Understanding the oil displacement by water through ultra-narrow pore throats presents an enormous challenge to experimental measurements since they cannot reveal the underlying mechanism in nano-scale. On the other hand,

the breakthrough pressure of oil displacement by water through pore throats has been widely described by the capillary pressure based on the Young-Laplace (Y-L) equation which is built upon a macroscopic perspective. While there have been a few molecular simulation works reported on the two-phase displacement process through inorganic pore throats with the throat widths down to 2 nm from a microscopic perspective, an explicit investigation of oil displacement by water through kerogen ultra-narrow pore throats has not been reported. In this work, we use molecular dynamics (MD) simulation to study oil (represented by octane) displacement by water through a 2-nm kerogen (represented by Type II-C kerogen) pore throat. We find that when the pressure difference between the upstream and downstream is lower than , water phase is stuck at the opening of kerogen pore throat, while the water-octane-kerogen interface curvature is dependent on . When , the water phase can displace the oil phase through the pore throat. Although the Type II-C kerogen is oil-wet based on water-oil-kerogen contact angle calculations, water has an excellent sweeping efficiency thanks to the hydrogen bonding between water and heteroatoms (such as O, N, and S) on kerogen surface. We also compared and from the Y-L equation with the contact angle and oil-water interfacial tension obtained from separate MD simulations on the water-octane-kerogen and water-octane systems, respectively. Surprisingly, from the widely used Y-L equation shows an excellent agreement with obtained from MD simulations for the 2-nm kerogen pore throat for a wide range of reservoir pressures. This work reveals underlying mechanism of oil displacement by water through an ultra-narrow kerogen pore throat from a microscopic perspective and provides important guidance to numerical modeling on oil recovery process in shale formations.

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MS3 / 425

## Oil recovery mechanisms in fractured tight carbonates by low-IFT foams

**Authors:** Xiongyu Chen<sup>1</sup> ; Kishore Mohanty<sup>2</sup>

<sup>1</sup> *University of Texas at Austin*

<sup>2</sup> *The University of Texas at Austin*

**Corresponding Authors:** mohanty@mail.utexas.edu, haplobasalt@gmail.com

Fracture systems exists in carbonate oil reservoirs with either natural or artificial origins. The permeability contrast between the fracture and the matrix makes most injection fluids bypass the matrix and result in low matrix oil recovery, especially for low-permeability matrices. Low IFT gas and foam injections can enhance oil recovery by decreasing capillary pressure and diverting gas from the fracture to the matrix. We use micro-coreflood experimentation and in-situ micro CT imaging to study the pore-scale mechanisms of gas-oil-water displacements in the fracture, at the fracture-matrix interface and within the matrix during gas and foam flows. In general, foam recovers additional oil in the matrix compared with gas injection and the matrix oil recovery increases with the decreasing gas-oil IFT. Foam ruptures at the fracture-matrix interface play a critical role for oil displacement in the matrix and are controlled by pore throat sizes and the gas-oil IFT. Last, oil displacement in the matrix by the near-miscible gas/foam flow benefits from the synergy of low-IFT capillary invasion and mass transfer across the gas-oil interface, which caused a uniform saturation profile in the radial direction of the matrix.

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Time Block C (18:00-21:00 CET) **References:**

Xiongyu Chen and Kishore K. Mohanty (2021), Pore-Scale Study of Oil Recovery by Gas and Foam in a Fractured Carbonate Rock at Different Gas–Oil Interfacial Tension, Energy & Fuels **Acceptance of Terms and Conditions:**

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MS25 / 721

## On Fuzzy-Systems Modeling of Subsurface Flow

**Authors:** Boris Faybishenko<sup>1</sup> ; Lavanya Ramakrishnan<sup>1</sup> ; Deborah Agarwal<sup>2</sup>

<sup>1</sup> *Lawrence Berkeley National Laboratory*

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**Corresponding Authors:** daagarwal@lbl.gov, bafaybishenko@lbl.gov, lramakrishnan@lbl.gov

Data sets collected from field or laboratory experiments for the determination of unsaturated hydraulic parameters—water retention curves and unsaturated hydraulic conductivity—are often uncertain, imprecise, incomplete or vague because of a vague delineation of subsurface heterogeneities and preferential flow zones. The other source of uncertainty is inconsistency between the real physical processes and the physics of the field and laboratory measurements. The use of soil physical and hydraulic parameters, which are commonly expressed using crisp relations, often leads to significant uncertainties in predictions.

One of the modern approaches to deal with uncertain data is the use of the fuzzy systems modeling. Fuzzy systems modeling, based on the application of the possibility theory, is a tool to evaluate the uncertainty of predictions of complex systems, given the uncertainty of input parameters. Possibility theory is concerned with event ambiguity, that is the extent to which some event occurs, given incomplete information expressed in terms of fuzzy propositions or fuzzy numbers.

The goal of this presentation is to present an approach to the prediction and uncertainty evaluation of hydrogeological systems based on a combination of the statistical and fuzzy-system modeling analyses. In particular, a rationale for representing heterogeneous soil and fractured rock systems as a fuzzy system will be presented. Fuzzy C-means clustering is applied to partition the 11 soil types of the UNSODA database into a series of overlapping clusters based on the fuzzy degree of membership. Fuzzy relations of the van Genuchten and Brooks-Corey unsaturated hydraulic parameters are derived, and these fuzzy relations are then applied for the fuzzy-systems time series predictions of the infiltration flux. Predictions are based on a fuzzy-form of Darcy's equation for unsaturated-saturated subsurface media. Fuzzy modeling techniques are well suited to utilize the imprecise input information for the uncertainty evaluation of predictions, risk assessment, and management of soil and hydrological systems.

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MS7 / 31

## On Modeling Nonlinear Flow and Reactive-Diffusion Processes in Heterogeneous Fractured-Porous Media



**Authors:** Boris Faybishenko<sup>1</sup> ; Jens Birkholzer<sup>1</sup>

<sup>1</sup> *Lawrence Berkeley National Laboratory*

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Experimental and theoretical studies indicate that nonlinear dynamical processes are inherent into flow and transport through fractured porous media. However, numerical predictions based on commonly applied numerical models using classical Darcy's, Richards' and Fick's concepts may significantly deviate from real transport processes in porous media. The goal of this paper is to demonstrate an application of several numerical reduced-order models, using systems of partial and ordinary differential equations, for simulations of hydro-chemical transport in heterogeneous fractured porous media: (a) Darcy-Brinkman (DB) equation for flow in porous media, given as a system of four ordinary differential equation, including a kinetic component related to fluid velocity, pressure, and gravitational potential, and (b) 1D and 2D Fisher-Kolmogorov-Petrovsky-Piskunov (FKPP) partial differential equations, which are used in chemistry, heat and mass transfer, biology and ecology to describe the coupled diffusion and reaction processes. The results of simulations of the DB equation demonstrate the transition of the flow pattern from steady convection to deterministic chaos and then to randomness. The simulations of the FKPP equation demonstrate how the degree of heterogeneity may change the concentration profile. An application of the Shannon's information entropy shows an asymptotic increase in the degree of complexity of the 2D modeling domain as the number of inclusions increases. The solutions of the fundamental DB and FKPP equations are important to improve our understanding of coupled physical-chemical subsurface processes and interactions in fractured-porous media, relating to petroleum and geothermal studies, environmental management and remediation, mining, gas storage, and radioactive waste isolation in underground repositories.

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MS6-B / 453

## On a coupled FE-formulation for the freezing process of ice within the framework of the TPM

**Authors:** Alexander Schwarz<sup>1</sup> ; Joachim Bluhm<sup>1</sup> ; Jörg Schröder<sup>1</sup>

<sup>1</sup> *University Duisburg-Essen*

**Corresponding Authors:** j.schroeder@uni-due.de, joachim.bluhm@uni-due.de, alexander.schwarz@uni-due.de

In this work, a coupled finite element method based on porous media theory (TPM), see e.g. 1 [2], for direct modeling of the phase transition of ice and water is presented. In detail, the presented model investigates ice deformation, temperature evolution, and the evolution of energy, enthalpy, and mass exchanges between its constituents. The main idea is based on a theoretically motivated evolution equation for the phase transition of ice and water, which guarantees thermodynamic consistency and is mainly determined by the local temperature rate, see e.g. [3], where it is assumed that the local temperatures of the phases are equal. The resulting finite element is a four-field formulation in terms of ice displacements, fluid pressure, volume fraction of ice, and temperature. Here, we use quadratic interpolation of the ice displacements and linear interpolation for the other degrees of freedom. The model is investigated in the context of first academic simulations of freezing processes of ice floes.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

1 R.M. Bowen. Incompressible porous media models by use of the theory of mixtures. *International Journal of Engineering Sciences* 18:1129-1148, 1980.

[2] R.M. Bowen. Compressible porous media models by use of the theory of mixtures. *International Journal of Engineering Sciences* 20:697-735, 1982.

[3] O. Coussy, Poromechanics of freezing materials, *Journal of the Mechanics and Physics of Solids* 53:1689-1718, 2005. **Acceptance of Terms and Conditions:**

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**Poster + / 719**

## **On compressibility error of the lattice Boltzmann method for pore scale modeling of non-Darcy flow**

**Authors:** Milad Hosseini<sup>None</sup> ; Majid Siavashi<sup>None</sup> ; Milad Shirbani<sup>None</sup> ; Mohaddeseh Mousavi Nezhad<sup>1</sup>

<sup>1</sup> *Associate Professor*

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Due to recent advances in imaging technology, calculating the macroscopic properties of a porous medium through pore-scale simulation has become very common. There are several methods to simulate pore scale flow patterns 1, [2]. Among those, lattice Boltzmann method (LBM) has been widely used by scientists because of its simple approach in modeling the complex pore space boundaries, a key challenge in pore-scale simulation [3]. One of the main concerns about the LBM is high compressibility errors that reduce the prediction capacity of the method at high Reynolds numbers. [4]. In this study, we have tried to minimize the prediction error generated by the variation of the compressibility via adjusting the solution conditions and without the need to refine the lattice size. This makes it possible to employ the LBM to reliably predict transition to the non-Darcy flow regime in real samples with complex pore structure. For this purpose, a multi-relaxation time collision model in the PALABOS library [5] is employed, and the fluid viscosity in the lattice unit is optimized. Thus, the effects of viscosity change on the bounce back boundary condition is minimize [6]. This enables us to predict the non-Darcy flow for fluids with LBM. Through these simulations it is concluded that the effect of the compressibility is significantly more important than the effect of the maximum velocity condition on the reliability of the LBM simulations.

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**MS9 / 699**

## **On pore scale simulation of reactive flows in the case of complex catalytic reactions**

**Authors:** Pavel Toktaliev<sup>None</sup> ; Oleg Iliev<sup>None</sup>

**Corresponding Authors:** oleg.iliev@itwm.fraunhofer.de, toktaliev@itwm.fraunhofer.de

Pore scale simulation of reactive flows is a challenging and computationally intensive problem, especially in the case of complex reactions. In many applications, the complicated chemical reactions are handled via coupling a transport solver to a proper software tool for chemistry, e.g., such as ChemKin, Phreeqc, Reactoro. The practice, however, shows that such simulations can be very time consuming, and often are subject to severe time step restrictions.

Furthermore, it is an open question when the upscaling of reactive flow through thin porous media (e.g., filter membrane) is possible. While there are a lot of discussions when this can be done for single phase flow depending on the size and number of pores, there is a lack of understanding in the case of passive and reactive transport through thin porous media. In a recent paper [1] a simulation of reactive transport in a 3D CT image of a piece of a wall of a catalytic filter was performed for the case of simple first order reaction. It was shown that the particular problem can not be upscaled and only pore scale simulations can help to understand the performance of the filter. Our goal is to investigate reactive flow in catalytic filters on synthetic geometries, as well as on 3D CT images of real geometries, in the case of complex reactions. The first step toward achieving this goal is to develop efficient algorithms for pore scale simulation in the case of complex reactions. Our current results on this task are the subject of this presentation. Results from the numerical simulation will be presented and discussed.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

1 R. Greiner, T. Prill, O. Iliev, B.A.A.L. van Setten, M. Votsmeier. Tomography based simulation of reactive flow at the microscale: Particulate filters with wall integrated catalyst. *Chemical Engineering Journal*, 378, 2019, 121919 **Acceptance of Terms and Conditions:**

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Poster + / 76

## On predicting pore fluid pressure changes in unsaturated porous media subject to undrained processes

**Author:** Angelica Tuttolomondo<sup>1</sup>

**Co-authors:** Alessio Ferrari<sup>1</sup>; Lyesse Laloui<sup>1</sup>

<sup>1</sup> EPFL

**Corresponding Authors:** lyesse.laloui@epfl.ch, alessio.ferrari@epfl.ch, angelica.tuttolomondo@epfl.ch

Predicting the induced change of fluid pressure in an unsaturated porous medium during undrained loading/unloading processes is challenging because two different fluids (a liquid and a gaseous solution) and a mixture of solid particles are involved. The relative presence of the two fluids and solid particles in the medium of interest, their stiffness, and the initial conditions in terms of liquid and gaseous pressure can play a crucial role in dictating the fluid pressures to be expected at the end of an undrained process. Knowledge of these pressure changes is essential because they affect the mechanical behavior of the porous medium, involving, for instance, its shear strength and volume. In this context, the analytical formulations of the so-called “pore pressure coefficients” proves to be a useful tool for making such predictions. A pore pressure coefficient is defined as the change in pressure of a fluid per unit change in total stress (the latter is the stress component of interest) (Lambe and Whitman, 1969). In contrast to existing models (Skempton, 1954; Hasan and Fredlund, 1980), this contribution proposes an analytical approach for determining unsaturated pore pressure coefficients, which adopts the generalized effective stress (Nuth and Laloui, 2008). It refers to an isotropic elastic unsaturated soil, and total stress changes under isotropic and oedometer conditions. It is shown that it is possible to define a unique pore pressure coefficient for an equivalent fluid. This has advantages in ensuring a direct transition between saturated and unsaturated state predictions. The proposed formulation also includes the analytical expression of the liquid-gas mixture stiffness; the latter is a function of the unique pore pressure and individual pore fluid coefficients. The number of constitutive parameters required for the applicability of the approach is lower than that needed to apply the currently existing approach for unsaturated soils (Hasan and Fredlund, 1980; Fredlund and

Rahardjo, 1993). The proposed formulation also makes it easy to define the change in the soil water retention state resulting from the undrained process. Existing results in the literature are interpreted or predicted, highlighting the advantages and suitability of the proposed methodology.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

Fredlund, D. G. & Rahardjo, H. (1993) Soil mechanics for unsaturated soils. New York, John Wiley and Sons.

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Nuth, M. & Laloui, L. (2008) Effective stress concept in unsaturated soils: Clarification and validation of a unified framework. International Journal for Numerical and Analytical Methods in Geomechanics 32(7):771-801. **Acceptance of Terms and Conditions:**

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MS24 / 193

## On the Equations of Nonlinear Single-Phase Poroelasticity

**Author:** Cornelis Johannes (Hans) van Duijn<sup>1</sup>

<sup>1</sup> *Eindhoven University of Technology*

**Corresponding Author:** c.j.v.duijn@tue.nl

In this presentation we consider the equations of nonlinear poroelasticity derived from mixture theory. They describe the quasi-static mechanical behavior of a fluid saturated porous medium. The nonlinearity arises from the compressibility of the fluid and from the dependence of porosity and permeability on the divergence of the displacement. We point out some limitations of the model. In our approach we discretize the quasi-static formulation in time and first consider the corresponding incremental problem. For this, we prove existence using Brezis's theory of pseudo-monotone operators. Generalizing Biot's free energy to the nonlinear setting we construct a Lyapunov functional, yielding global stability. This allows us to construct bounds that are uniform with respect to the time step. If dissipative effects between the fluid and the solid are taken into account, resulting in an additional time derivative, we obtain the continuous time case in the limit when the time step tends to zero. This yields existence of a weak free energy solution. This is joint work with Andro Mikelić to whom this mini-symposium is dedicated.

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MS6-B / 589

## On the effects of colloidal particles in controlled oil-water interfaces.

**Authors:** Mario Cordova-Gonzalez<sup>1</sup> ; S. H. Hejazi<sup>1</sup>

<sup>1</sup> *University of Calgary*

**Corresponding Authors:** mario.cordovagonzale@ucalgary.ca, shhejazi@ucalgary.ca

The flow of colloidal particle suspensions in multiphase systems have become widely studied in applications such as oil recovery, drug delivery, and contaminant transport. In oil extraction processes, about two-thirds of the original oil in place remains underground after primary or secondary production. An important key factor contributing to the deficiency of recovery methods is the heterogeneity of the oil reservoirs. The morphology of the porous medium is heterogeneous with many distinct pore configurations, both in size and shape. For instance, oil may get trapped in cavities (dead-end pores) connected to conductive channels. The inherent geometrical restriction of a dead-end pore configuration inhibits the possibility to liberate the trapped fluid by displacement methods. Nanoscale particles placed at oil-water interfaces may produce a more uniform and elastic interfacial configuration when subjected to deformation. This elasticity may help oil to be drained from cavity confinements. Most nanoscale particles are either hydrophilic or hydrophobic and do not settle at the interfaces. Enabling particles to be surface activate by means of physicochemical interactions with natural surfactant molecules present in the crude oil such as asphaltenes, resins, and organic acids is a provident and not well-documented alternative.

In this work, we examine the in-situ particle activation at the oil-water interfaces subjected to a shearing flow field. We fabricate microfluidic chips with a well-defined pattern consisting of a main flow channel connected to multiple dead-end pores. We orchestrated a displacement methodology in which fumed silica particles in a carrier aqueous solution bypass a series of cavities saturated with an oil phase doped with surfactant. The interactions of silica suspensions at 1, 2, and 4 wt.% concentrations and oil-soluble surfactants above critical micellar concentrations are examined. We use a color camera and a confocal laser scanning microscopy to monitor and visualize the displacement process. We measure the dilatational interfacial viscoelasticity and dynamic interfacial tension of oil-water systems by means of a drop shape analyzer and the Spinning Drop Tensiometer.

The results show that notable particle-coated water-oil interfaces developed in the presence of surface-active particles. When dispersed particles on injecting water enter cavities saturated with the trapped micellar solution, oil in water emulsions at the oil-water interface are instantaneously formed. As water penetrates the cavity area, the residual oil films left behind the interface interact with the particles in the aqueous phase forming rigid and well packed micro-size droplets. The growth of the emulsion zone in cavities is a function of oil viscosity and decreases as the oil viscosity increases. A relationship between the oil-water interfacial viscoelasticity, dynamic interfacial tension, surfactant and particle concentrations, oil viscosity spontaneous in-situ emulsification, and consequently oil discharge from cavities is established and discussed.

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**Poster + / 408**

## **On the inverse problem of identifying the effective pore size distribution using non-Newtonian fluids**

**Author:** Martin Lanzendörfer<sup>1</sup>

<sup>1</sup> *Charles University, Prague*

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In contrast to water (as a Newtonian fluid), the flow of some non-Newtonian fluids through porous media is related to the geometry of the pores in a way that allows to backtrack some information,

such as the approximate distribution of the effective pore sizes. This can be (and has been) done in various ways, cf. the yield stress fluid porosimetry method (YSM), based on the yield stress fluid model, or more recently the model by Abou Najm and Atallah (ANA model), based on shear-thinning fluid models. The core of these methods consists of the mathematical inverse problem that needs to be solved numerically. As usual for the inverse problems, challenges may arise.

Some sets of experimental data may not reveal any information about the pore sizes. Some data may lead to numerically ill-posed problems. We do not know how the measurement error affects the inverse problem results. How to plan an optimal set of the flow experiments? After all, the two methods mentioned above focus on two distinct features of what can be the very same fluid, such as an aqueous solution of xanthan gum or guar gum, while subject to either very low (YSM), or considerably larger (ANA), shear rates. The approach which we follow attempts to cut the problem into pieces that should be first considered separately. Some of the issues can be studied by using the numerical experiments with artificial data based on the idealized capillary bundle forward problem, or on the flow through some simplified pore space geometry.

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MS4 / 75

## On the mechanical behavior of expansive porous media with consideration on chemical effects

**Author:** Angelica Tuttolomondo<sup>1</sup>

**Co-authors:** Alessio Ferrari<sup>1</sup>; Lyesse Laloui<sup>1</sup>

<sup>1</sup> EPFL

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Experimental geomechanics highlights that the mechanical behavior of expansive porous media is variable depending on the pore water chemical composition. These porous media are typically characterized by clay particles, whose activity (Skempton, 1953) (and thus propensity to expand) is itself dependent on the pore water chemical composition. Chemical-induced mechanical effects on both shear strength and volumetric behavior are highlighted in the literature (Di Maio, 1996; Castellanos et al., 2008). The physical-chemical origin of this mechanical dependence is still debated. Consequently, geomechanical approaches that can properly include these effects are still limited. The possibility of using a generalized effective stress concept for the mechanical modeling of these materials is an attractive proposition with the following advantages (Nuth and Laloui, 2008): (i) assured transition between saturated and unsaturated states, (ii) uniqueness of the critical state line irrespective of the degree of saturation, (iii) direct inclusion of hydraulic effects and corresponding hysteretic characteristics. In this contribution, we first account for the solid particle-pore water interaction and distinguish the different types of ions and water characterizing expansive porous media (Tuttolomondo et al., 2021). Also, we highlight how the presence of both movable and non-movable ions is essential in defining the pore water chemical composition. Second, we provide an analytical approach for determining the pore water pressure and replace the specified expression in the generalized effective stress definition. The effective stress also depends on a chemical variable related to the interaction between the solid particles and the pore water. The water retention curve (describing the evolution of matric suction at varying degree of saturation) and the effective solute suction curve (representing the evolution of the introduced chemical variable at varying degree of saturation) are essential to account for the retention state of the material and the chemical composition of the pore water at any state of interest. Existing experimental results in the literature, both at saturated and unsaturated conditions, are reinterpreted to investigate the advantages of the proposed geomechanical approach. The results obtained highlight, among others, the following additional benefits when

using the proposed extension of the generalized effective stress concept: (i) the uniqueness of the failure envelope irrespective of the pore water chemical composition; (ii) the possibility of predicting elastic strain induced by pore water chemical composition changes (Tuttolomondo et al., 2021). Combined with the provided physico-chemical explanation, these results bring the basis for an advanced stress-strain constitutive modeling.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

Castellanos, E., Villar, M. V., Romero, E., Lloret, A. & Gens, A. (2008) Chemical impact on the hydro-mechanical behaviour of high-density FEBEX bentonite. *Physics and Chemistry of the Earth, Parts A/B/C* 33:S516-S526.

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Tuttolomondo, A., Ferrari, A. & Laloui, L. (2021) Generalized effective stress concept for saturated active clays. *Canadian Geotechnical Journal*. **Acceptance of Terms and Conditions:**

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#### Student Poster Award:

MS25 / 732

## On the value of using electrical resistance tomography to enhance sub-surface heterogeneity representation in HYDRUS 2D for simulating solute transport at the hillslope scale.

**Authors:** Nandita Gaur<sup>1</sup> ; Maria Teresa Tancredi<sup>1</sup> ; David Radcliffe<sup>1</sup> ; Binayak Mohanty<sup>2</sup>

<sup>1</sup> *University of Georgia*

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Solute transport modeling at the hillslope scale warrants a detailed soil domain description. This is true even if we expect only matrix flow since variations in soil layering, like differences in the depth to impeding layer, could alter the location where preferential flow processes like funnel flow occur. The traditional pedological soil horizon-based representation may be inadequate to represent such processes and thus lead to incorrect transport dynamics such as travel time even if the average signature of solute concentration is adequately represented. On the other hand, there is a trade-off to an increased representation of heterogeneity which is the problem of equifinality. In this study, we compare a parsimonious genetic horizon based model with a detailed model to assess the value of increasing heterogeneity representation for modeling transport of a conservative solute (chloride) at the hillslope scale. The study site is located in the Piedmont region of Georgia that is characterized by deep saprolite and variable bedrock depth. We developed the detailed model by estimating a high resolution soil texture map of the hillslope that was derived using soil electrical resistivity in an Artificial Neural Network (ANN) framework. The ERT driven soil layering model uses three easily measured inputs: soil resistivity, relative depth of investigation, and weekly antecedent rainfall. To train and test the model, we used soil samples, collected in 30-cm increments up to 510 cm, from 11 different locations across a 42 m hillslope transect. Texture was measured using a laser particle size analyzer. We used bootstrapping to train and test the ANN framework to identify the minimum set of soil samples required to generate an acceptable dataset and concluded that models trained on 6 locations had the least uncertainty. The soil texture predictions had values of  $R^2=0.74$  and  $RMSE=0.4$ . From the obtained textures, we created a hillslope domain in HYDRUS 2-D to predict hydrological and chloride transport at the hillslope scale. Both models are calibrated using water table elevations. In this presentation, we will discuss the soil texture determination process from ERT and the key differences in calibration and predictions for the two hydrologic models.

**Time Block Preference:**Time Block C (18:00-21:00 CET) **References:****Acceptance of Terms and Conditions:**Click here to agree **Newsletter:**I do not want to receive the InterPore newsletter **Student Poster Award:**

MS3 / 157

**Online Fast Flow simulations for Discrete Fractured Media with Non-Standard Reduced Basis Method****Authors:** Fabio Vicini<sup>1</sup> ; Stefano Berrone<sup>2</sup><sup>1</sup> *Politecnico di Torino*<sup>2</sup> *Politecnico di Torino, Italy***Corresponding Authors:** fabio.vicini@polito.it, stefano.berrone@polito.it

Reduced Basis (RB) methods are well-known and widely used techniques applied to complex parameterized simulation problems to obtain reliable discrete results for a particular choice of parameters, largely reducing the computational time to obtain the numerical solutions.

Flow simulations in underground fractured media seems to be a perfect application for the RB framework, due to the stochastic nature of the mechanic properties and the complex geometries of the domain obtained by random probability distributions.

Unfortunately, standard RB tools proved to be ineffective in the robust PDE-constrained optimization formulation proposed in [1], because of the use of non-conforming meshes for the computation of the underground flow on Discrete Fracture Network (DFN).

Thus, with the help of the residual-based a posteriori error available in [2], we propose an aggregated trial reduced space [3] reduced with an alternative RB greedy technique which requires no inf-sup lower bound estimation.

Numerical tests will be presented to show the ability of the technique to recover the right RB space dimension with a smart stopping criterion which relates the accuracy of RB approximation with the accuracy of the high fidelity solution.

**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:**

1 S. Berrone, A. Borio, and F. Vicini. Reliable a posteriori mesh adaptivity in discrete fracture network flow simulations. CMAME, 2019.

[2] S. Berrone, S. Scialò, and F. Vicini. Parallel meshing, discretization, and computation of flow in massive discrete fracture networks. SISC, 2019.

[3] F. Negri, G. Rozza, A. Manzoni, and A. Quarteroni. Reduced basis method for parametrized elliptic optimal control problems. SISC, 2013 **Acceptance of Terms and Conditions:**

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Poster + / 405

**Operator Splitting with Capillary Relaxation (OSCAR)****Author:** Julien Maes<sup>1</sup><sup>1</sup> *Heriot-Watt University*



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Direct modelling of multiphase flow in pore structures at the micron-scale and at low capillary number is challenging for two reasons. Firstly, numerical error in the modelling of interface curvature and surface tension force leads to large spikes in velocity called spurious currents. Secondly, accurate and robust modelling of capillary waves requires small time-steps based on the Brackbill conditions, often orders of magnitude smaller than stable time-steps required by CFL conditions. In this work, we investigate how a novel time-stepping method based on operator-splitting method, and labelled OSCAR, can be employed to perform simulations at low capillary numbers. OSCAR splits the Navier-Stokes system of equations for two-phase flow in viscous and capillary relaxation steps. The viscous steps are performed with large time-steps based on the CFL number, while the capillary relaxation steps are performed with smaller time-steps based on the Brackbill condition. We perform a range of simulation on three different geometries (e.g. straight microchannel, micromodel, constriction) and we observe that at capillary numbers lower than  $10^{-5}$  and as low as  $10^{-9}$ , the capillary relaxation steps converge well before the global time-step has been reached, leading to orders of magnitude reduction in the computational time. However, spurious currents play a major role here too, as they may prevent convergence of the capillary relaxation steps and can lead to a large increase of CPU time. Our investigation shows that it is essential to tackle time-stepping and spurious currents simultaneously in order to perform fast and accurate simulation of multiphase flow at low capillary numbers.

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MS8 / 291

## Optimal Fluid Stretching for Mixing-limited Reaction in Rough Fracture Flows

**Authors:** Seonkyoo Yoon<sup>1</sup> ; Marco Dentz<sup>2</sup> ; Peter Kang<sup>3</sup>

<sup>1</sup> *University of Minnesota, Twin Cities*

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<sup>3</sup> *University of Minnesota*

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Mixing-induced reactions occur when two or more reactive species physically come into contact, and the interplay between fluid stretching and diffusion has a critical role in inducing the contact. Mixing-induced reactions in channel flows are of great interest in numerous engineering applications and natural processes, including microfluidics, biomedical devices, and fracture flows. In many of these applications, predicting the spatiotemporal evolution of chemical reactivity is critical. Here, we demonstrate that such prediction is possible through the concept of optimal fluid stretching that enables us to predict the locations of reaction hot spots.

We study the reactive displacement of two miscible fluids in rough channel flows over wide ranges of Péclet number (Pe) and channel roughness. At the mixing interface, the two fluids react according to the instantaneous irreversible bimolecular reaction  $A + B \rightarrow C$ . We simulate the advection-diffusion-reaction problem using a random walk based reactive particle method that is free of numerical dispersion. The relative contribution of stretching and diffusion to mixing-limited reaction is controlled by changing the Péclet number (Pe), and the channel roughness is also systematically varied. We observe optimal ranges of fluid stretching that maximize reactivity, which are captured by a Lagrangian measure based on an effective time period that honors the stretching history. We show that the optimality originates from the competition between the enhanced mixing by fluid stretching and the mass depletion of the reactants. We analytically derive the spatial distribution of

reaction products using a lamellar formulation and successfully predict the optimal ranges of fluid stretching, which are consistent across different levels of channel roughness. These findings provide a mechanistic understanding of how the interplay between fluid stretching, diffusion, and channel roughness controls mixing-limited reactions in rough channel flows, and show how reaction hot spots can be predicted from the concept of optimal fluid stretching.

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MS25 / 600

## Optimal Irrigation control in Richards Equation Framework

**Author:** Marco Berardi<sup>1</sup>

**Co-authors:** Fabio Difonzo<sup>2</sup>; Roberto Guglielmi<sup>3</sup>

<sup>1</sup> *Consiglio Nazionale delle Ricerche - Istituto di Ricerca sulle Acque*

<sup>2</sup> *University of Bari - Department of Mathematics*

<sup>3</sup> *University of Waterloo*

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In this work we investigate a tool for optimizing the amount of water necessary for an efficient irrigation. In particular, we propose an optimal control approach for suitably handling top boundary conditions in Richards' equation, in a 1D spatial domain. The minimization problem of the given objective functional aims at optimizing the root water uptake term while minimizing the amount of water provided in the irrigation process.

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Poster + / 553

## Optimising site selection for hydrogen storage in porous rocks in the North Sea & Irish Sea

**Author:** Lubica Slabon<sup>1</sup>

<sup>1</sup> *University of Edinburgh*

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Hydrogen for clean energy is in the national and international spotlight. Offshore wind presents an extensive renewable energy source in the UK, and a large green hydrogen resource, positioning the UK to be a major player in the emerging global hydrogen market. In the UK and around the globe

there's a handful of likely subsurface hydrogen storage sites and it is widely recognised that hydrogen storage in porous media (rocks) will be necessary to support the scale of production, storage and use anticipated for a global hydrogen economy.

A key component of subsurface risk management is the suite of geological controls needed to ensure that storage is efficient and secure (i.e. that injected fluids do not leak from the storage formation). The project will characterize, translate and test a suite of geological controls (including caprocks and hydraulic barriers) and explore the sub-processes which govern their ability to trap hydrogen. The aims is to better understand hydrogen flow through porous media (rocks) and hydrogen behavior in underground settings. In order to achieve the goal, the first approach was to map possible distribution of hydrogen density within the North Sea. A database of pressure, temperature, salinity and depth measurements for 191 gas and oil reservoirs within the North Sea was collected. Hydrogen density, brine density and buoyancy was calculated in order to understand its special variation in relation to pressure and temperature distribution. Sensitivity analysis were carried out to understand relationship and influential extent between the selected parameters.

Understanding of geological controls is critical to inform the selection of appropriate reservoir sites as well as designing safe and effective storage and recovery schemes. The project outcomes will inform (a) criteria to site selection, monitoring and assessment approaches for hydrogen geological storage, and (b) potential for engineered barriers for enhanced containment or leak remediation.

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Poster + / 6

## Optimizing gradient functional material for enhanced performance of solar-driven thermochemical fuel production

**Authors:** Da Xu<sup>1</sup> ; Meng Lin<sup>1</sup>

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Porous media is the key energy conversion media in two-step solar thermochemical fuel production devices. The conventional way of fabricating porous metal oxide structure shows limited flexibility in varying local morphology for better transport properties. The material structure optimization is hindered by lack of methodology precisely tuning material structure and lagged modeling framework to assess the structure-property relationship of designed materials. This structure-property knowledge can be further linked to the final solar-to-fuel efficiency of reactors using such material. The triply periodic minimum surface (TPMS) structures are promising candidates due to their flexible lattice structure design, well-defined analytical expression, and easiness in anisotropic feature introduction. Moreover, the recent development of direct ceramic 3D printing technologies enables a unique route for the fabrication of gradient functional materials with complex structures.

In this study, we focused on the optimization of TPMS structures' transport properties and their impacts on the thermochemical behaviors. Volume-averaged TPMS morphological properties, radiative transfer properties, as well as effective mass and heat transfer properties are evaluated by a comprehensive in-house modeling framework. The transport properties obtained was then used in continuum multi-physics model for the evaluation of the thermal and thermochemical performance of a cylindrical cavity reactor. The model was validated with a complete discrete model at pore-level. Via screening TPMS structures' under various design geometrical parameters, design guidelines for macro-structure of porous reacting media for thermochemical fuel process will be provided.

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**Poster + / 116**

## PORE-SCALE MODELLING IN SUPPORT OF SAFETY ASSESSMENT STUDIES FOR NUCLEAR WASTE REPOSITORIES IN FRACTURED ROCK

**Authors:** Paolo Trinchero<sup>1</sup> ; Aitor Iraola<sup>1</sup> ; Patrick Bruines<sup>2</sup> ; Martin Stigsson<sup>2</sup> ; Bjorn Gylling<sup>3</sup> ; Jan-Olof Selroos<sup>4</sup>

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Safety assessment (SA) studies for spent nuclear fuel repositories in fractured rock entail the need to account for very large spatial and temporal scales. This is typically done by using continuum-based or Discrete Fracture Network (DFN)-based numerical simulations, which in turn rely on upscaled groundwater flow and transport parameters. However, model parameterisation is sometimes based on gross simplifications and there are still open questions such as: (i) what is the role of fracture filling minerals for flow channelling? (ii) what is the influence of mineral precipitation/dissolution processes on the evolution of flow channelling and on radionuclide transport including retention? and (iii) what is the impact of the altered rim zone bordering flowing fractures on radionuclide uptake by matrix diffusion? Here, we show how pore-scale simulations are used to address such questions and thus provide the basis for a more consistent derivation of effective parameters for use in large-scale SA simulations. The pore-scale models are based on a realistic yet synthetic single fracture that was generated using fractal theory<sup>1</sup> and later imported followed by meshing using the open software OpenFOAM (<http://www.openfoam.org>). Calcite filling patches, which are typically found in field observations on drill-cores<sup>2</sup>, were subsequently generated using Sequential Indicator Simulations (SIS) carried out using the geostatistical software SGeMS<sup>3</sup>. Groundwater flow through the partly-filled fracture was computed using a Darcy-Brinkman-Stokes formulation<sup>4</sup> and the ingress through the inlet of a slightly acidic unsaturated solution was simulated. The results show that the dissolution of calcite patches leads to a gradual increase of the fracture flow wetted surface area (i.e. the area of the fracture in contact with the flowing water) as well as a gradual increase of groundwater flow rates. In terms of retention capacity, due to diffusion in the matrix, the system shows a progressive decrease of the F-factor<sup>5</sup> (i.e. the ratio between the flow wetted surface area and the groundwater flow rate), which is consistent with an alternative interpretation based on the integration of the transport resistance<sup>6</sup> along transport pathways traced at different simulation times. We will also show the results of an on-going project, where a limited part of the fracture has been extracted and the bordering rock matrix included explicitly. The aim of this model is to study the effect of thin alteration rims on matrix diffusion processes.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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- (2) Löfgren, M.; Sidborn, M. Statistical Analysis of Results from the Quantitative Mapping of Fracture Minerals in Forsmark: Site Descriptive Modelling-Complementary Studies; R-09-30; Svensk kärnbränslehantering (SKB), 2010.
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Pore-Scale Perspective. *J. Fluid Mech.* 2017, 827, 457–483. <https://doi.org/10.1017/jfm.2017.499>.

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**Poster + / 598**

## Parametrization of uncertainty for predictive modeling of subsurface flow problems

**Author:** Alsadig Ali<sup>1</sup>

**Co-authors:** Abdullah Al-Mamun<sup>2</sup>; Marcio Borges<sup>3</sup>; Maicon Correa<sup>4</sup>; Felipe Pereira<sup>1</sup>; Arunasalam Rahunanthan<sup>5</sup>

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<sup>2</sup> *United International University*

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We are concerned with a Bayesian framework for rock characterization consisting of a preconditioned Markov chain Monte Carlo (MCMC) method in conjunction with a truncated KL 1 expansion for the parametrization of the underlying uncertainty in subsurface properties [2]. Reduction of the overall uncertainty in determining reservoir characteristics can be achieved through the incorporation of static (e.g., measurements of rock properties at sparse locations) and dynamic data (e.g., saturation values at sparse locations or production curves) in the characterization framework.

In this work we focus on the generation of conditional random fields, that honor known values of the permeabilities at given locations (static data). The model problem considered is the two-phase immiscible displacement with unfavorable viscosity ratio in a heterogeneous reservoir. Initially we review currently available procedures for incorporating sparse measurements in truncated KL expansions. We show that they may produce unwanted inaccuracies in the prediction of subsurface flows. Motivated by these results we propose a novel, projection-based conditioning procedure that overcomes the difficulties that have been identified, and show that the new procedure produces accurate predictions while taking into account sparse measurements of rock properties.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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[2] A. Al-Mamun, J. Barber, V. Ginting, F. Pereira, A. Rahunanthan, Contaminant transport forecasting in the subsurface using a Bayesian framework, *Applied Mathematics and Computation* 387 (2020) 124980. **Acceptance of Terms and Conditions:**

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MS13 / 663

## Particle Flow Through a Hydrophobic Nanopore

**Author:** Kim Kristiansen<sup>1</sup>

**Co-author:** Signe Kjelstrup<sup>2</sup>

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Sparked by the interest in hydrophobic membranes for use in membrane distillation for the purification of water by means of thermally driven transport of water from impure liquid phase to a purified vapour phase, we provide the beginnings of an analytical model for the full range of transport coefficients for gas flow through porous media where the solid phase interacts with the fluid by a repulsive force. We focus here on the transport properties of a hydrophobic nanopore of cylindrical geometry. A model for a more general porous medium may then be given as a statistical distribution of such pores. While Knudsen diffusion of rarefied gases in small cylindrical pores, isothermal as well as non-isothermal, is a well-studied phenomenon, we provide an analytical model to assess the effect of a repulsive interaction between the gas particles and the pore walls. Isothermal transport of rarefied gases has seen some recent advances in this direction [1], as well as the non-isothermal case for slip flow [2]. We provide here clear physical interpretations of the effects of the repulsive interaction on the non-isothermal transport of gas through a pore, and discuss how this knowledge can be applied to the design of porous materials optimized for a particular purpose.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

1 Bhatia et al. Molecular transport in nanopores: a theoretical perspective. *Phys. Chem. Chem. Phys.*, 2011, 13, 15350-15383.

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MS15 / 585

## Particle transport and filtration in 2D and 3D porous media: coupling CFD and Deep Learning

**Author:** Agnese Marcato<sup>1</sup>

**Co-authors:** Gianluca Boccardo<sup>1</sup>; Daniele Marchisio<sup>1</sup>

<sup>1</sup> *Politecnico di Torino*

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The study of particle transport in porous media is a research field of great interest as it is involved in a wide variety of applications [1]. The random nature of porous media systems makes it difficult to analytically correlate the impact and the synergy of their geometrical parameters. Since these features make these systems a suitable candidate for machine learning (ML) approaches, in our work we employed neural networks for the realization of data-driven models. These techniques are able to grasp non-linear correlations between data and to account for a large number of input parameters. Moreover in the case of convolutional neural networks the entire system geometry can be used as input for the model, in this way it is possible to avoid the selection of the geometrical features [2-3]. In this work we coupled computational fluid dynamics (CFD) simulations with machine learning

models. The results of a CFD simulations campaign are employed as a training set for the neural networks in order to obtain a computationally inexpensive data-driven surrogate model which is able to replace the CFD simulation, while keeping a good accuracy. The aim of the CFD investigation is the flow, transport, and filtration at the pore-scale, in this framework the first step is the creation of the geometries. We designed bi-dimensional [4] and three-dimensional [5] periodic packings of spheres via the open-source framework YADE DEM.

For each kind of geometry, hundreds of simulations are solved, each differing randomly in their geometrical parameters and input operating conditions. The CFD simulations are performed on the open-source code OpenFOAM. At first, the fluid flow is evaluated in the limit of small Reynolds numbers ( $<0.1$ ), thus obtaining the medium permeability. Then the transport of dilute colloid particles is studied by solving the advection-diffusion equation, and the filtration rate is calculated [6].

Two kinds of models have been built: both for the prediction of the permeability of the porous media, and the filtration rate of the colloid through the grains. The first one is a simple fully-connected neural network whose input features are the geometric parameters and operating conditions. The second one is a convolutional neural network whose input is a porous medium geometry, in the form of a binary matrix. After the neural network training process, the end result is a surrogate black-box model capable of predicting the output values when given a new set of input features, or a new geometry; notably, the accuracy of this data-driven model is on-par or better than other analytical or empirical correlations.

This simple data-driven models can then be reliably used in place of expensive CFD simulations (or in general, all “first principles” methods), as one single call of the neural network has a computational cost which is orders of magnitude lower than the full CFD simulation: in our test problems, under a second versus several hours – with a total neural network training time of around four minutes, for the fully connected one, and of several hours, for the convolutional one.

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MS6-B / 549

## Pattern formation controlled by friction and viscous forces in deformable granular media

**Authors:** DAWANG ZHANG<sup>1</sup> ; Bjornar Sandnes<sup>1</sup>

<sup>1</sup> Swansea University

**Corresponding Authors:** b.sandnes@swansea.ac.uk, 936575@swansea.ac.uk

We study the invasion patterns when injecting the water with the injection rate of different magnitude into a layer of dry hydrophobic beads contained in a Hele-Shaw cell. We observed a decrease of characteristic finger width with the increase of granular volume fraction, an increase of number of fingers invaded simultaneously with the increase of injection rate, and an increase of finger width with the increase of the flow rate inside the finger. The invasion patterns are reproduced in simulation, and the theoretical models to explain and predict these observations are developed.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS24 / 406

## Patterns in a reaction-diffusion double porosity system

**Authors:** Mikhail Panfilov<sup>1</sup> ; NOURA EDDAOUTI<sup>2</sup>

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We study the behaviour of a system of equations that describes diffusion with chemical reactions caused by microorganisms in a double porosity medium. The objective is to find various classes of nontrivial limit solutions at large time (the patterns), especially simultaneous spatial-temporal patterns. In contrast to a classical reaction-diffusion system (RDS), our system contains four reaction-diffusion equations (RDE) describing the transport of nutrients and the dynamics of bacteria in fractures and blocks, with exchange terms. This system occupies an intermediate place between the Turing's RDS, which can have only spatial or temporal patterns separately, and a wavy RDS, which can have simultaneous spatial-temporal patterns in the form of standing waves. We show analytically, for a reduced version of the system, that spatial-temporal patterns can exist but in another form than a standing wave. The full system has been analysed numerically. Among with known patterns, we have detected a nontrivial simultaneous spatial-temporal pattern that has the form of travelling flashes. They correspond to the Hopf-Andronov temporal oscillations in blocks and to Turing's spatial fluctuations in fractures.

There results have been used to analyse the behaviour of an underground storage of hydrogen. We show several different scenarios of the evolution of such a storage and discuss the optimal regime.

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MS25 / 416

## Pedotransfer for infiltration estimation

**Authors:** Yakov Pachepsky<sup>None</sup> ; Seongyun Kim<sup>1</sup> ; Gülay Karahan<sup>2</sup>

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Recently progress in the international infiltration studies has been stimulated and summarized by Harry Vereecken and colleagues in several international efforts. These developments created opportunities to expand the knowledge on infiltration to large-scale projects by developing pedotransfer functions for infiltration equations. The complexity of relationships between parameters of infiltration equations and readily available soil and landscape data calls for the use of machine learning methods for the PTF development. This work's objective was to run a pilot project on pedotransfer for infiltration with the data from large international Soil Water Infiltration Global (SWIG) database and address the following questions:

1. Can soil basic properties and land-use inform about the most appropriate infiltration equation and, if yes, then what are the most influential predictors?
2. Can soil basic properties and land-use be used as predictors of infiltration equations' parameters, and if yes, then does the accuracy of the parameter estimation depend on the accuracy?

Research with 1830 SWIG datasets showed that which infiltration equation will perform the best depends on the input soil properties and land use domain. Inputs that predicted the Horton, Kostiaikov-Lewis (Mezencev) equation being the best, provided more reliable predictions than inputs that pointed to Green-Ampt, Philip, and Swartzendruber equation being the best. The infiltration measurement method was a dominant predictor, and using the textural class provided the accuracy of predicting the best equation comparable with using the silt, sand, and clay contents. The accuracy of predicting Horton and Mezencev equations' parameters did not depend on the performance of these equations. This accuracy strongly depended on the infiltration measurement method. Further research is needed to understand how to establish the threshold to consider the accuracy of two equations different. Also, the dependence of pedotransfer accuracy on affected by the observed infiltration stages needs to be studied. Overall, opportunities exist to provide additional means for infiltration modeling in multiple applications.

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## Peltier Heats in Lithium-Ion Batteries

**Author:** Astrid Fagertun Gunnarshaug<sup>1</sup>

**Co-authors:** Lena Spitthoff<sup>2</sup> ; Preben Joakim Svela Vie<sup>3</sup> ; Odne Burheim<sup>2</sup> ; Signe Kjelstrup<sup>1</sup>

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Temperature is known to be of importance for the ageing, performance, and safety of lithium-ion batteries. The heat released or absorbed inside a battery has therefore been a topic of much interest. The heat released or absorbed with the cell reaction, the reversible heat effect, is commonly included in thermal models through the entropy change of the reaction. The total reversible heat is then distributed evenly over the cell. However, the cell reactions are occurring at the two electrode interfaces resulting in two local effects known as the Peltier heats. 1

An anodic electrode surface reaction with a positive Peltier heat will be cooling down, while a negative Peltier heat means it is heating up. For lithium-ion batteries this means that an electrode which heats during discharge, will cool during charging. The two local Peltier heats combine under the assumption of isothermal conditions to give the entropy change of the reaction. [2] If the entropy change is small, the Peltier heat of the individual electrode surfaces may still be large. [1,2] In such a situation one electrode surface would cool while the other heats. To distribute the reversible heat effect uniformly, would therefore give an inaccurate temperature profile.

We will show how entropy measurements of lithium-ion batteries with a lithium metal counter electrode can be used to predict the Peltier heats of electrode materials of various chemistries and lithium content if the Peltier heat of Li-metal is known. These data are already available in literature [3,4] and has heretofore been unexploited. We will see that one electrode surface will cool while the other releases heat. [5] The importance of these local effects will be for the temperature profile on a single-cell level and a stack will shown. 1

#### Acknowledgment

The authors are grateful to the Research Council of Norway through its Centres of Excellence funding scheme, project number 262644, PoreLab.

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## Permeability Decay Evaluation for a Nonlinear Oil flow through Porous Media in a Wellbore Near a Sealing Fault through Green's Functions (GF's)

**Author:** Fernando Bastos Fernandes<sup>1</sup>

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Nonlinear oil flow through porous media near a sealing fault has a key role in reservoir engineering because the existence of sealed zones in many types of reservoir rocks present in the world. This

work proposes a new unsteady 2-D permeability pore pressure-dependent model for a wellbore near a sealing fault, where analytical solution is based on an integro-differential solution of the Nonlinear Hydraulic Diffusivity Equation (NHDE) through Green's Functions (GF's). The model also considers the variation in the properties of the rock and the fluid present inside its pores. The unsteady 2-D pressure field is described by the sum of two exponential integral functions  $E_i(xD, yD, tD)$ , that constitute a combined flow (radial, near to the wellbore) and linear (near to the sealing fault). This type of flow in geosciences and petroleum engineering literature is known as pseudo-radial flow. Authors also implement the new model in Matlab® software in order to evaluate the general solution, so as initial and boundary conditions. The model calibration is performed through a porous media oil flow simulator, which showed a high convergence. The permeability functions for some types of reservoir rock are obtained through laboratory correlations, generated from synthetic field data. Authors conclude that general solution of NHDE is given by the sum of line-source solution  $PwD(tD)$  and the first order term of the series asymptotic expansion,  $mWD(1)(tD)$ . This second term of the series expansion is obtained by solving a Volterra's second kind integro-differential equation in Matlab and is responsible for all the nonlinearities of the combined oil flow. Results of this research showed that when the fault presence begins to contribute to the pressure drop at the well, the drawdown data increasingly departs from the semilog straight line. After a long transitional period, a second straight line with slope 2m can be noticed. Authors also realized that the pressure graphs showed excellent agreement when compared to a numerical simulator and presented errors less than 0.5%.

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## Permeability Prediction via 3D Convolution Neural Networks

**Authors:** Mohamed Elmorsy<sup>1</sup> ; Wael El-Dakhakhni<sup>2</sup> ; Benzhong Zhao<sup>3</sup>

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Subsurface fluid flow prediction is critical in many natural and industrial processes such as groundwater movement, oil extraction, and geological carbon dioxide sequestration. These processes are controlled by the permeability of the underground porous media (i.e., soil, rock, etc.). Traditionally, the permeability of porous media is determined via expensive and labor-intensive lab-based methods. More recently, advances in digital rocks technology have enabled permeability prediction via computational fluid dynamics simulations. However, these simulations remain computationally demanding and time consuming. These complications are barriers to characterizing subsurface media in a fast and efficient way, limiting direct flow simulation of porous media to only samples of few millimeters in size. Here, we present an efficient, data-driven model based on 3D Convolution Neural Networks (CNNs) that learns the morphological and topographical features of porous media from CT images and makes permeability predictions. Specifically, our model is capable of predicting the permeability of real porous media samples from only geometry input (end-to-end) in as few as 4 milliseconds with a low error cost (~10%).

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## Perturbation Theory for Fluids under Confinement

**Authors:** Vilde Bråten<sup>1</sup> ; Daniel Tianhou Zhang<sup>1</sup> ; Morten Hammer<sup>2</sup> ; Ailo Aasen<sup>3</sup> ; Sondre Kvalvåg Schnell<sup>4</sup> ; Øivind Wilhelmsen<sup>2</sup>

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Perturbation theory based equations of state (EOS) have the ability to provide insight on the behavior of model fluids, which makes them useful tools in thermodynamics. One of these is the Baker Henderson perturbation theory (BHPT) 1. It uses the hard sphere fluid as a reference system, and is known to provide accurate predictions for macroscopic pure-component fluids at high temperatures. Small systems are known to deviate from the classical thermodynamic description, which means that a macroscopic EOS will fail to predict the properties of a small system [2]. For fluids confined in small geometries, there is therefore currently a lack of successful methods to predict thermodynamic properties from EOS.

We show how the BHPT can be modified to accurately predict the behavior of fluids under confinement. The extended theory is referred to as BHPT-small. Crucial to this method is the definition of the “bulk” density of a small system, and the behavior of the radial distribution function (RDF). Two major findings were made by investigating how the RDF of a hard sphere fluid, confined by a spherical geometry differs from the bulk RDF. Due to the non-periodic boundaries of the confined system, the RDF will approach zero for at indefinitely pair-distances, instead of tending towards unity. In addition, particles adsorb on the boundary of the spherical confinement, which leads to a depletion of particles in its center. The density experienced by the particles in the center is therefore not equal to the average density of the fluid.

We further demonstrate how BHPT-small can be formulated for pores of different sizes and shapes. The extended perturbation theory provides a tool to compute thermodynamic properties of nanosystems that is applicable to a variety of examples.

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## Pesticide transport in unsaturated soils: from column tests to laboratory lysimeter.

**Authors:** Luca Vetere<sup>1</sup> ; Monica Granetto<sup>1</sup> ; Carlo Bianco<sup>1</sup> ; Roberto Revelli<sup>1</sup> ; Rajandrea Sethi<sup>1</sup> ; Tiziana Tosco<sup>1</sup>

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Raising crop production and at the same time reducing environmental spreading of agrochemicals are two current priorities in agriculture. Balancing these needs a quantitative understanding is needed of infiltration phenomena and agrochemical leaching into the subsoil. To this aim, field studies are undoubtedly the most reliable approach to retrieve representative data. Lysimeters are specific devices installed in fields used for studying percolation of water and, to a lesser extent, of contaminants through the unsaturated zone (Howell et al., 1991). However, full-scale detailed monitoring of water infiltration and more importantly leaching of chemical substances may be complex. To overcome this problem, laboratory flow and transport tests in small scale soil-packed columns (typical size, few cm in diameter, 10 to 20 cm in length) have been traditionally applied to study into details key processes controlling, in general, solute transport (Dontsova et al., 2006), and more specifically the effects of agrochemical applications (Masipan et al., 2016). However, under some circumstances, the reduced size may limit the representativeness of the results, and up-scaling to the field could be limited. This work aims at linking these different experimental scales via a set of infiltration tests performed at three different laboratory scales, namely small columns (1.6 cm in diameter, 11 cm long), intermediate columns (10 cm in diameter, 25 cm long), and laboratory lysimeter (30 cm in diameter, 70 cm long), all packed with the same porous medium (Dorfner silica sand for a set of tests, and a Lufa standard soil for another set). Water flow and transport tests of solutes and of a pesticide (Dicamba) have been carried out to investigate the differences among the scales in terms of operating conditions, hydrodynamic dispersivity, hydraulic conductivity, pesticide interaction with the soil. The transport tests have been performed applying the solute or Dicamba to the top of the columns, followed by a flushing with water (mimicking irrigation and rain events). Injection rates have been properly selected at the three scales to have the same Darcy velocity, thus ensuring comparability. Outflow water has been collected and analyzed at all scales to reconstruct the breakthrough curve. Moreover, in the lab lysimeter, water content, matric potential, pH, EC and ORP have been measured at different depths for a correct reconstruction of the flow field, concentration profiles and breakthrough curves. The experimental data have been fitted using HYDRUS to obtain unsaturated flow and transport parameters. Dicamba showed little interaction with the soil at all scales, and results are comparable among all setups, suggesting that even small columns can be representative of large-scale processes provided that operating conditions are properly selected, even though large-scale setups are necessary while investigating the influence of unsaturated flow in the top soil on pesticide leaching.

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## Phase Transitions in Disordered Mesoporous Solids: Effect of Geometric Disorder

**Authors:** Henry Enniful<sup>1</sup> ; Daniel Schneider<sup>2</sup> ; Dirk Enke<sup>2</sup> ; Rustem Valiullin<sup>3</sup>

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Majority of porous solids used in industrial processes such as energy storage, separations and catalysis possess structural disorder over varying length scales. These disorder effects strongly affect the properties of the confining fluids in the pores. Hence, detailed quantification of structural disorder with correlation to fluid phase behavior is a necessary step towards optimization for practical applications.

Employing the serially connected pore model (SCPM), we have determined the impact of a number of disorder-related parameters, including effect of pore chain length, “powder effect” and interconnectivity effect on phase transitions in disordered mesopore spaces. Additionally, we have showed experimental results from solid-liquid phase transitions obtained by NMR cryoporometry and gas-liquid transitions observed from nitrogen sorption experiments to corroborate the theoretical predictions from the SCPM.

We conclude that, the SCPM has the potential of explaining many features of experimentally observed phase transitions in disordered mesoporous solids.

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## Phase behavior of a confined ionic discotic liquid crystal

**Author:** Mohamed Kolmangadi<sup>1</sup>

**Co-authors:** Andreas Schoenhals<sup>1</sup> ; Sabine Laschat<sup>2</sup> ; Patrick Huber<sup>3</sup>

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Liquid crystalline mesophases in nanoconfinement exhibit intriguing orientational order and phase transition behaviors. Here, the plastic crystal to hexagonal columnar, and hexagonal columnar to isotropic transition temperatures are studied for the guanidinium-based ionic discotic liquid crystal confined in self-ordered nanoporous alumina membranes. The phase transition temperature of the plastic crystal to hexagonal columnar phase is reduced with inverse pore diameter. The hexagonal columnar to isotropic transition is suppressed completely in all pores and a possible explanation is given. The results are of technological relevance for the design of liquid crystal-based devices such as batteries and sensors with optimum tunable properties

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## Phase field fracture propagation with proppant transport and two phase flow

**Authors:** Sanghyun Lee<sup>1</sup> ; Andro Mikelic<sup>None</sup> ; Mary Wheeler<sup>2</sup> ; Thomas Wick<sup>3</sup>

<sup>1</sup> *Florida State University*

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In this talk, we present an extension of the phase-field fracture propagation model to the immiscible two-phase flow fracture model, and with a transport problem. The flow model is derived by using the lubrication theory, and we provide the absolute and relative permeabilities with nonzero capillary pressure. The contribution in solid mechanics consists of displacements and a phase-field variable. Both systems are coupled employing a fixed-stress splitting and discretized by employing continuous Galerkin finite element methods. The flow and transport system has resident and injected pressures and saturations, and concentration of transported species. The flow problem is treated with a locally conservative enriched Galerkin finite element method to provide accurate flux to the transport problem. Modeling and algorithms are substantiated with several numerical tests.

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## Phase-field modelling of bulk-surface PDEs and adhesive interfaces

**Authors:** Anne Boschman<sup>1</sup> ; Matteo Icardi<sup>1</sup> ; Kristoffer G. van der Zee<sup>1</sup> ; Bindi S. Brook<sup>1</sup> ; Federico Municchi<sup>None</sup>

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In a wide range of porous media applications, the evolution of material boundaries is driven by complex processes at the interface such as biofilm growth and surfactant dynamics, or between two interfaces such as adhesion. To describe and understand these multi-phase and bulk-surface interactions we make use of phase-field modelling. Within this framework, we will present a new and thermodynamically-consistent model for adhesion, for instance between one of the fluid phases and a non-moving porous medium. A coupling term is introduced into the free energy to account for the adhesive interaction. The resulting adhesion model is a stiff, higher-order, non-linear partial differential equation, which needs to be solved using an energy-stable time-integration scheme. In addition, to further incorporate interfacial dynamics, e.g. those in biofilm growth, a surface partial differential equation can be solved using the diffuse interface approach. In this contribution, we will discuss the underlying foundations of our model in terms of thermomechanical consistency and present some preliminary numerical results-oriented towards porous media applications.

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## Phase-wise conservative and physics-preserving algorithms for multi-phase flow in porous media

**Author:** Shuyu Sun<sup>1</sup>

**Co-authors:** Huangxin Chen<sup>2</sup> ; Haijian Yang<sup>3</sup>

<sup>1</sup> *King Abdullah University of Science and Technology (KAUST)*

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Modeling and simulation of multiphase flow in porous media have been a major effort in reservoir engineering and in environmental study. One basic requirement for accurate modeling and simulation of multiphase flow is to have the predicted physical quantities sit within a physically meaningful



range. For example, the predicated saturation should sit between 0 and 1 while the predicated molar concentration should sit between 0 and the maximum value allowed by the equation of state. Unfortunately, popular simulation methods used in petroleum industries do not preserve physical bounds. Another major issue with common algorithms for two-phase flow, especially common semi-implicit algorithms, is that they are (locally) conservative to just one phase only, not all phases.

In this talk we present our work on both fully implicit and semi-implicit algorithms for two-phase and multi-phase flow in porous media with capillary pressure. Our proposed algorithms are locally mass conservative for all phases. They are also able to accurately reproduce the discontinuity of saturation due to different capillary pressure functions, and the produced total velocity is continuous in the normal direction. Moreover, the new schemes are unbiased with regard to the phases and the saturations of all phases are bounds-preserving (if the time step size is smaller than a certain value for semi-implicit algorithms). We also present some interesting examples to demonstrate the efficiency and robustness of the new algorithms. The semi-implicit algorithms are based on our novel splitting of variables, and the fully implicit algorithms are based on the two nonlinear preconditioner of active-set reduced-space method and nonlinear elimination, as well as the linear preconditioner of overlapping additive Schwarz type domain decomposition. The semi-implicit part of this presentation is based on our joint work with Huangxin Chen (Xiamen University), Jisheng Kou (Shaoxing University), Xiaolin Fan (Guizhou Normal University), and Tao Zhang (KAUST), and the fully implicit part is based on our joint work with Haijian Yang (Hunan University), Chao Yang (Beijing University), and Yiteng Li (KAUST).

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## Physics Impact on Deep Neural Networks for Multiphase Flow in Porous Media

**Authors:** Bicheng Yan<sup>1</sup> ; Dylan Harp<sup>1</sup> ; Bailian Chen<sup>1</sup> ; Rajesh Pawar<sup>2</sup>

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Many recent studies have demonstrated the superior predictive interpretability and physics consistency by anchoring deep feedforward neural networks (DNN) with physics laws. As this type of network is fully connected, it potentially suffers low training efficiency when predicting complex problems such as multiphase flow in porous media.

In this study, we propose a learning framework to predict the state variables of pressure, saturation and well flow rate in fluid flow in porous media. Since fluid flow in porous media is constrained by physics, we allow the learning framework to flexibly intake either pure labeled data, or a combination of labeled data and physics data in terms of governing equation or physics-based operators. Given that the loss evaluation of non-labeled data during backpropagation is expensive due to automatic differentiation, a modified batch-mode training procedure with transfer learning is proposed to ensure that it balances the training efficiency and the contribution of all the samples on the training loss. As well flow rates are time series data only associated with well locations, it is effectively predicted along with pressure and saturation by a simple sparse operator in the same framework.

Numerical experiments of multiphase flow related to geologic carbon storage are used to gauge the performance of learning framework. Our results show that DNN integrating labeled data with physics or the physics-based operators doesn't bring too much additional CPU cost due to automatic

differentiation, but they effectively improves the fidelity of pressure and saturation prediction compared to DNN with labeled data only. Moreover, the prediction of the well flow rate is quite accurate with average error lower than 2.0%. Therefore, the learning framework helps us to investigate the impact of physics on DNN predictions, and provides us the guidance to effectively train a DNN with a good combination of physics and labeled data.

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## Plants control soil gas exchanges possibly via mucilage

**Author:** Adrian Hauptenthal<sup>1</sup>

**Co-authors:** Mathilde Brax<sup>2</sup> ; Jonas Bentz<sup>2</sup> ; Hermann Jungkunst<sup>2</sup> ; Klaus Schützenmeister<sup>2</sup> ; Eva Kröner<sup>1</sup>

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Gaseous matter exchanges in soil are determined by the connectivity of the pore system which is easily clogged by fresh root exudates. However, it remains unclear how a hydrogel (e.g. mucilage) affects soil pore tortuosity when drying. The aim of this study is to obtain a better understanding of gas diffusion processes in the rhizosphere by explaining patterns formed by drying mucilage.

We measured oxygen diffusion through a soil-mucilage mixture after drying using a diffusion chamber experiment. Therefore we mixed soil with different particle size with various amounts of mucilage. Afterwards we saturated the soil and measured the gas diffusion coefficient during drying.

We found that mucilage decreases gas diffusion coefficient in dry soil without significantly altering bulk density and porosity. Electron microscopy indicate that during drying mucilage forms filaments and interconnected structures throughout the pore space. Exudation of mucilage may be a plant possibility to actively alter gas diffusion in soil.

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**MS9 / 167**

## Plug size pore network extraction with pore scale resolution

**Authors:** Clément Varloteaux<sup>1</sup> ; Mohamed Regaieg<sup>None</sup> ; Titly Farhana Faisal<sup>2</sup> ; Igor Bondino<sup>3</sup>

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When dealing with pore scale simulation, two main methods are generally used: direct numerical simulation (DNS) and Pore Network Modeling (PNM). The former can use different formalism like Lattice-Boltzmann, Navier-Stokes or Smooth-Particle-Hydrodynamics. While DNS can provide more precise results than PNM, it cannot get reliable results on multiphase flow on images exceeding  $500^3$  voxels. On the other hand, PNM allows to reach much wider volumes at the cost of precision. Lately, Raeini et al. (2017) have proposed a hybrid solution that can get profit from both DNS and upscaling through a Pore Network Model where properties of the network are determined from DNS by solving Stokes equation on the segmented image.

However, the extraction code that can produce such a network is limited by the memory of the machine, especially when dealing with large volumes (network extraction from a two billion voxels 3D image needs more than 128Gb of memory). To overcome this limitation, a stitching process has been developed on networks extracted from overlapping sub-volumes of a given image. Then, simulations on the large extracted network are held by the TOTAL's pore-scale network simulator DynaPNM (Regaieg et al. 2021).

In this talk, the stitching method is first presented. Then, a validation process for both qualitative and quantitative evaluation of the discrepancy introduced by the stitching process, for both single and two phase flow, is proposed. Guidelines on the input parameter choice for stitching are exposed, justified by a sensitivity study. Three rock-types are used as source materials for these studies (one outcrop and two reservoir rocks). Moreover, strategies to get a cubic pore network from a source image with a large aspect ratio are discussed.

Finally, the application on centimeter long rock samples is presented on an extracted pore network representing a rock volume up to  $46\text{cm}^3$  (equivalent to a large  $10000 \times 8000 \times 8000$  voxel image scan at a voxel resolution of  $4\mu\text{m}$ ).

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Poster + / 397

## Poiseuille viscous flows in menisci-bounded “bridges” and crevices of triangular pore channels: Blunt’s model revisited

**Author:** Anvar Kacimov<sup>None</sup>

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We consider Blunt’s 1 pore as a straight cylindrical conduit of a triangular cross-section OO1O2. A viscous liquid bridge is bounded by menisci AMD and CNB which are assumed to be circular arcs of radii,  $r_1$  and  $r_2$ , only slightly varying in the  $f$ -direction perpendicular to Fig.1a.

Fig.1

The contact angle  $\theta/2$ . Flow in the  $f$ -direction (Fig.1b) is caused by the longitudinal gradient of pressure,  $p$ , in the bridge (like in [3]). This gradient emerges due to, for instance, increase of the disjoining and capillary pressure inside the liquid due to gradual “thinning” of the bridge (owing to, say, decrease of  $r_2$  and increase of  $r_1$ ). In application to evaporation of water in vertical isothermic porous columns (vadoze zone above a horizontal water table), the evaporation-induced “thinning” of the bridge is determined by a higher evaporation rate from the menisci of larger diameters (near the water table), as compared with the drier soil surface where the moisture content in desert sands

is small and, therefore, the sizes of the water-filled crevices and menisci radii are tiny. We introduce Cartesian coordinates and get the Poisson equation:

(1)

where  $u$  is velocity in the  $f$ -direction,  $\mu$  is the liquid's viscosity and  $e = \text{const}$ . The flow domain,  $G_z$ , in Fig.1c is made of two straight segments DC and BA and two arcs AMD and CND. The boundary conditions are:

(2)

where  $\theta$  is an angular coordinate counted from the axis of symmetry of the bridge, i.e. OMN. The air phase is of zero viscosity. BVP (1), (2) is solved by the methods of complex analysis [2,3]. From this solution we get the vector field  $u$ , flow rate through the bridge,  $Q(a, e, r_1, r_2) = \int_{G_z} \mu u(x, y) d^2x$ , and permeability of various bundles of triangular capillaries laden with bridges.

Fig.2

We also consider a right triangular conduit with an immobile air entrapped near the three vertices (O, O1, O2) in Fig.2a. Three identical menisci there are circular arcs of a constant radius  $r_1$ ;  $G_z$  is a circular sextagon bounded by these menisci and three no-slip segments. We consider a curvilinear pentagon  $Dz = ADECEEB$ , where E is the centre of the pore and EC and EB are the midpoints of the sides OO1 and OO2. Along EC EEB the shear stress is zero. If  $r_1$  is small enough (soil is close to full saturation), then the corner EC EEB of the pentagon is approximated by a circular arc. One circular arc of a radius  $r_{2m}$  can be drawn via points EC and EB and another, of a radius  $r_{2M}$  – via point E (Fig.2a, dotted line) that gives two domains,  $D_m$  and  $D_M$ . These two bounding tetragons geometrically sandwich the curvilinear pentagon  $Dz$ . Hence, the maximum principle for Poisson's equation (1), yields a double inequality  $Q_m < Q_z < Q_M$ . Therefore, our analytical solution to BVP (1), (2) also approximates one for  $Dz$  in the case of in Fig.2a. Similarly, a viscous gas flow along the core of a pore channel with an "entrapped" water in the three crevices (Fig.2b) is studied.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS21 / 443

## Population balance models for particulate flows in porous media: breakage and shear-driven events

**Authors:** Nicodemo Di Pasquale<sup>1</sup>; Daniele Marchisio<sup>2</sup>; Matteo Icardi<sup>3</sup>

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Population Balance Equation (PBE) successfully describes particle evolution in different flow conditions (Di Pasquale et al., 2012). However, despite predictive macroscopic models for polydisperse particulate flows are relevant for many Porous Media (PM) applications (Municchi and Icardi, 2020; Municchi et al., 2020) such as subsurface (water, oil) reservoirs and industrial filtration, there is still

limited use of the PBE framework in the PM community. In this talk, we will explore a general population balance model for particle transport at the pore-scale, including aggregation, breakage and surface deposition. Using dimensional analysis, we analyse the different terms in the equations and we here propose to split the various mechanisms considered in the PBE to describe the evolution of a population of particles into one-and two-particles processes. While the former are linear processes, they might both depend on local flow properties (e.g. shear). This observation has important consequences for the problem we are considering, since the upscaling (via volume averaging and homogenisation) to a macroscopic (Darcy-scale) description now requires closures assumptions. Here, we show how to obtain such closures for specialised cases, pure breakage without aggregation caused by shear forces on the transported particles. We obtain, in arbitrary periodic geometries, accurate models for the upscaled breakage and collision frequencies, starting from non-linear power-law dependence on the local fluid shear rate. Results are presented for a two-dimensional channel flow and a three dimensional regular arrangement of spheres, for arbitrarily fast (mixing-limited) events. This work represents the foundation of a new general framework for multiscale modelling of particulate flows in porous media.

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## Pore Connectivity Analysis and Electrical Conductivity Model for Tight Sandstones

**Author:** Xiaowei Zhang<sup>1</sup>

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Non-Archie's law phenomenon, where the saturation exponent varies with the water saturation, has been observed for tight sandstones due to bimodal pore size distribution and high clay content. In the study, we proposed a new method to analyze pore connectivity by multi-scale imaging techniques and established dual-porosity conductivity model for tight sandstones. Firstly, broad ion beam scanning electron microscope (BIB-SEM) is applied to acquire 2-D grayscale images with a resolution of 100 nm. Pores and main minerals are identified by image segmentation and cluster labelling algorithm. We classify the pores of tight sandstones into residual intergranular pores and intercrystallite pores that occur in clays. Secondly, dried samples with a diameter of 5 mm are imaged by a micro CT with a resolution of 3  $\mu\text{m}$ . The porosity resolved by the micro CT is far less than helium porosity measured in lab. The resolved pores form isolated clusters due to the absence of sub-resolved throats. The samples are saturated with sodium iodide solution and scanned by the micro CT to obtain 3-D grayscale images. Image registration methods are carried out on the two kinds of grayscale image. We find that the CT-resolved pores are mostly saturated by the solution. Furthermore, part of voxels standing for clay minerals in dried samples is invaded by the sodium iodide solution. It suggests that intercrystallite pores in clays are the main conductive paths in tight sandstones. The large intergranular pores are connected through the intercrystallite pores. Finally, a dual-porosity electrical conductivity model is established according to the result of pore connectivity analysis. The conductivity model of tight sandstones is built by combining series-parallel conductivity theory and W-S

argillaceous sandstone conductivity theory. The contributions of fluid in multi-scale pore space and surface conductivity of clay minerals on bulk electrical conductivity are both included. We predict the conductivities of the tight sandstone samples of the Ordos Basin using the dual-porosity model based on the measured porosity, clay content, and NMR T2 distribution. The calculated electrical conductivities agree well with the experimental results.

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MS19 / 11

## Pore Graded Anodic Transport Layers in PEM Electrolysers: A Pore Network Study

**Author:** Haashir Altaf<sup>1</sup>

**Co-authors:** Nicole Vorhauer<sup>2</sup>; Evangelos Tsotsas<sup>3</sup>; Tanja Vidakovic-Koch<sup>4</sup>

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Porous structures have widespread importance in electrochemical processes. The specific morphology of the available porous materials, as well as their physical properties, crucially affect their applications, e.g. their use in fuel cells, batteries, or electrolysers. A key point is the correlation of transport properties (mass, heat, and charges) in the spatially—and in certain cases also temporally—distributed pore structure. In electrolysers, the drainage of oxygen through a water-saturated porous transport layer (PTL) significantly impacts the performance of the overall system [1][2]. The oxygen coverage of the catalyst layer obstructs the water supply towards the reaction zone; this can lead to a decrease in the rate of reaction. In more detail, the oxygen produced at the catalyst layer must be removed through the PTL in a way that the water supply adequately persists. Mathematical modelling is used to investigate the impact of the PTL pore structure on the distribution of wetting (water) and non-wetting phase (oxygen). For this purpose, pore network models (PNMs) together with upscaling strategies are applied [3]. PNMs conceptually represent the porous media. Micro computed tomography is used to extract the required information, e.g. porosity and pore size distribution, pore connectivity, pore shape etc. The model uses this information to generate an interconnected network of pores. Relevant two-phase flow physics are used to study the transport limitations at microscale. With the help of PNM, it is studied how a change of structure, i.e., the spatial grading of the pore size distribution and porosity, changes the transport properties. Several situations are investigated, including a vertical gradient ranging from small to large pore sizes and vice versa, as well as a dual-porosity network extracted from a commercial PTL. The simulation results indicate that the specific porous structure has a significant impact on the spatial distribution of species and their respective relative permeabilities. In more detail, it is found that the continuous increase of pore sizes from the catalyst layer side towards the water inlet interface yields the best transport properties among the investigated pore networks. This outcome could be useful for the development of grading strategies, specifically for material optimization for improved transport kinetics in water electrolyser applications and for electrochemical processes in general.

**Time Block Preference:**

**Time Block A (09:00-12:00 CET) References:**

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**Poster + / 64**

## **Pore Pressure Sensitivity-Permeability Decay Evaluation for Non-linear Oil Flow in Porous Media through Green's Functions (GF's)**

**Author:** Fernando Bastos Fernandes<sup>1</sup>

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The unsteady nonlinear oil flow in porous media makes hydraulic diffusivity equation (HDE) harder to solve analytically and numerically. This work proposes a porous media formation damage evaluation caused by the permeability decay as function of pore pressure. To evaluate this phenomenon, a new integro-differential analytical model using Green's functions (GF's) is proposed to solve nonlinear hydraulic diffusivity equation (NHDE) for radial oil flow with source term. Model considers the change in the properties of the rock and the fluid present inside reservoir rock pores in respect to pore pressure. Normally, dimensionless wellbore solution  $PwD(tD)$  for slightly compressible flow of liquids in cylindrical coordinates is solved using the Laplace transform or Boltzmann transformation, obtaining an unsteady pressure profile described by the exponential integral function  $Ei(rD, tD)$ . Authors also implement the new model in Matlab® software in order to evaluate general solution, so as initial and boundary conditions. The model calibration is performed by comparing the solution obtained for pore pressure-dependent permeability with the solution through a porous media flow simulator and permeability functions for some types of reservoir rock are built through laboratory correlations, generated from synthetic field data. Authors conclude that general solution of NHDE is given by the sum of line-source solution  $PwD(tD)$  and the first order term of the series asymptotic expansion,  $mwD(1)(tD)$ . This second term of the series expansion is obtained by solving a Volterra's second kind integro-differential equation in Matlab and is responsible for all the nonlinearities of the flow. Results of the pressure graphs showed excellent agreement when compared to a numerical simulator and presented errors less than 0.5%.

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MS11 / 140

## Pore Scale Visualization of CH<sub>4</sub>-CO<sub>2</sub> Mixed Hydrates Phase Transitions During Stepwise Depressurization

**Author:** Jyoti Shanker Pandey<sup>1</sup>

**Co-authors:** Ørjan Strand<sup>2</sup>; Nicolas von Solms<sup>1</sup>; Geir Ersland<sup>2</sup>; Stian Almenningen<sup>2</sup>

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In this study, we investigate the dissociation pattern of CH<sub>4</sub>/CO<sub>2</sub> mixed hydrate in porous media using high-pressure micromodel. We formed CH<sub>4</sub>/CO<sub>2</sub> mixed hydrate from gaseous CH<sub>4</sub> and liquid/gaseous CO<sub>2</sub> to mimic the scenario where a CH<sub>4</sub> hydrate reservoir has been injected with CO<sub>2</sub>. Direct visualization was carried out using a high-pressure, water-wet, silicon-wafer based micromodel with a pore network of actual sandstone rock. Mixed hydrate was formed at reservoir conditions (P = 44-75 bar and T = 1.7-3.6°C) from either a two-phase system (liquid water and CH<sub>4</sub>/CO<sub>2</sub> gas mixture) or a three-phase system (liquid water, CH<sub>4</sub> gas, and liquid CO<sub>2</sub>).

A stepwise pressure reduction method was applied to record multiple dissociation pressure points for a given mixed hydrate system, and the molar concentration of CH<sub>4</sub>/CO<sub>2</sub> corresponding to each dissociation point was calculated. The effect of hydrate and fluid saturation on fluid flow during dissociation was also analyzed.

The results showed that liberated gas during stepwise pressure reduction was trapped by surrounding hydrate, and reformation of CO<sub>2</sub> hydrate occurred rapidly when liquid water was present. The reformed CO<sub>2</sub> hydrate shielded the CH<sub>4</sub> hydrate that was still not dissociated and complete dissociation was accomplished when the pressure was brought below the stability pressure of pure CO<sub>2</sub> hydrate.

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MS6-B / 442

## Pore network modeling of bubble ripening in porous media

**Authors:** Yashar Mehmani<sup>1</sup>; Ke Xu<sup>2</sup>

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The evolution dynamics of trapped bubble populations inside a porous medium through Ostwald ripening is relevant to several applications including CO<sub>2</sub> sequestration, liberation of bubbles from liquid hydrocarbons, methane hydrate formation, and oxygenation of groundwater aquifers. We present a pore network model that is capable of simulating the microscopic evolution of thousands



of trapped bubbles inside a porous material. The physics that govern the process include dissolution, capillary equilibrium, molecular diffusion, and geometric and topological characteristics of the confining solid. The competition between these physics leads to a rich array of macroscopic observations that are undecipherable from examining the microscopic governing equations alone. We validate the model against recent microfluidic experiments and then deploy it to predict the thermodynamic stability of trapped bubbles in heterogeneous media. Computational and algorithmic considerations key to achieve numerical stability will be highlighted.

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MS12 / 698

## Pore scale modelling of elastic properties of hydrate bearing sediment based on high resolution synchrotron x-ray computed tomography imaging

**Authors:** Rui Li<sup>1</sup> ; Yingfang Zhou<sup>2</sup> ; Wenbo Zhan<sup>1</sup> ; Jianhui Yang<sup>3</sup>

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Gas hydrate contains abundant methane and is expected to be a promising energy supply to mitigate the influence of climate change in the future, in addition, it is also relevant to geological hazards. Understanding the effect of fluids-solid-hydrate spatial distribution on elastic properties of hydrate-bearing sediments benefits the interpretation of the Bottom Simulating Reflection and acoustic logging data.

The elastic properties of gas hydrate-bearing have been investigated with various approaches, such as lab-based measurements and analytical models. But these methods fail to capture the influence of detailed pore structure and phase distribution on elastic properties. Alternatively, pore-scale imaging technologies (e.g., Sahoo, et al., 2018), has been used to understand the detailed pore-scale fluids-solid-hydrate distribution on the elastic wave properties. But pore-scale numerical simulation of elastic properties based on high resolution detailed fluids-solid-hydrate images is still rare.

In this work, effective elastic properties of gas hydrate-bearing were simulated by the finite element method based on high-resolution synchrotron x-ray computed tomography imaging. The results show that the dominant hydrate morphology experiences a transition from pore-filling to pore-bridging and to cementation during the hydrate formation process. Remarkably, some hydrate forming in small pores can cement adjacent granules and form local pore-bridging, which increases the rock elastic moduli and sonic wave velocities significantly even when hydrate saturation is low.

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**Reference:**

Sourav K. Sahoo, B. N. Madhusudhan, Hector Marín-Moreno, Laurence J. North, Sharif Ahmed, Ismael Himar Falcon-Suarez, Tim A. Minshull, and Angus I. Best. Laboratory insights into the effect of sediment-hosted methane hydrate morphology on elastic wave velocity from time-lapse 4-d synchrotron x-ray computed tomography. *Geochemistry, Geophysics, Geosystems*, 19(11):4502–4521, 2018. **Acceptance of Terms and Conditions:**

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MS21 / 143

**Pore scale two-phase simulation of viscous fingering of non-Newtonian fluids****Authors:** Takshak Shende<sup>1</sup> ; Vahid.J Niasar<sup>None</sup> ; Masoud Babaei<sup>2</sup><sup>1</sup> *The University of Manchester*<sup>2</sup> *University of Manchester***Corresponding Authors:** masoud.babaei@manchester.ac.uk, vahid.niasar@manchester.ac.uk, takshak.shende@postgrad.manchester.ac.uk

The direct numerical simulation of non-Newtonian fluids (modelled using shear stress-dependent Meter model) displacing oil in 3D Mt. Simon sandstone and 2D porous medium were conducted on heterogeneous media, and over a range of wettabilities (strong imbibition to strong drainage), capillary numbers and viscosity ratios. This study suggests that, compared to water flooding, viscous fingering can persist or be suppressed depending on the heterogeneity of porous media. It is very important to account for the microscale heterogeneity of porous media to design polymer solution injection.

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**Pore-Scale Imaging of Tertiary Controlled-Salinity Waterflooding in a Heterogeneous Carbonate Rock at Reservoir Conditions****Author:** Ahmed Selem<sup>None</sup>**Co-authors:** Nicolas Agenet<sup>1</sup> ; Martin Blunt<sup>2</sup> ; Branko Bijeljic<sup>3</sup><sup>1</sup> *TOTAL S.A.*<sup>2</sup> *Imperial College London*<sup>3</sup> *Imperial College***Corresponding Authors:** nicolas.agenet@total.com, b.bijeljic@imperial.ac.uk, a.selem18@imperial.ac.uk, m.blunt@imperial.ac.uk

Over the last decade multiple studies have shown the significance of controlled salinity water-flooding (CSW) as an efficient technique to improve recovery from oil fields. Most of the published experimental work in the literature was performed at the core scale and mainly focused on comparing the incremental oil recovery from low salinity (LS) and high salinity (HS) brine injection in secondary or tertiary modes. Wettability alteration towards a more water-wet state is believed to be the prominent effect of LS on reservoir rocks. However, the underlying pore-scale mechanisms responsible for the CSW effects are not fully understood especially in heterogeneous carbonate reservoirs.

In this work, we investigated pore-scale oil displacement and rock wettability in tertiary LS waterflooding (LSW), i.e. injecting LS brine at HS waterflooding (HSW) residual oil saturation. X-ray

micro-computed tomography (micro-CT), combined with a high-pressure high-temperature flow apparatus, was used to image in situ CSW on an Estailades limestone core sample (6 mm in diameter and 12 mm in length). To establish the wettability conditions found in oil reservoirs, the sample was aged for three weeks at 11 MPa and 80°C. The moderately oil-wet sample was then injected with HS brine at a range of increasing flow rates, namely at 1, 2, 4, 11, 22 and 42  $\mu\text{L}/\text{min}$  with 10 pore volumes injected at each rate. Subsequently, LS brine was injected following the same procedure. A total of 8 micro-CT images, with a resolution of 2.3  $\mu\text{m}/\text{voxel}$ , were acquired throughout LS and HS waterflooding. These images were utilised to characterize fluid configurations in the pore space and obtain saturations and occupancy maps. Pore space was quantified by micro-CT resolved porosity of 12.5% and sub-resolution micro-porosity of 17.0%. Wettability was characterised by measurements of in-situ contact angle and curvature.

The results showed that LSW has yielded an incremental oil recovery of 9% of OIIP, based on fluid saturations values measured on resolved macro-pores. The mean contact angle and curvature values showed insignificant changes with HSW; the measured mean curvature and the associated capillary pressure values remained negative. However, with LSW the capillary pressure increased towards a positive value, as the wettability progressed towards a mixed-wet state. The pore and throat occupancy analysis revealed a salinity-induced change in fluid distribution in the pore space. HS brine invaded mainly the larger pores and throats, but as LS brine was injected the fraction of medium- and small-size pores and throats occupied by oil decreased.

Overall, our analysis showed that a shift from a weakly oil-wet towards a mixed-wet state was observed mainly after low salinity brine was injected into the sample, hence the increase in oil recovery. This approach helped further investigate pore-scale wettability alteration in carbonates and enhanced the understanding of LSW as enhanced oil recovery method for potential field-scale applications.

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MS18 / 707

## Pore-Scale Investigation of Nano-Enhanced Chemical Strategy for In-situ Crude Oil Contaminated Soils Remediation

**Author:** Zahra Sakhaei<sup>1</sup>

**Co-authors:** Najmeh Ghorbani Saadatabadi<sup>1</sup>; Ehsan Nikoee<sup>2</sup>; Masoud Riazi<sup>1</sup>

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In recent decades, the problem of soil pollution by crude oil and other petroleum-derived fuels, has faced growing attention due to the quick urbanization and industrialization. Unfortunately, petroleum hydrocarbons-contaminated soil is causing significant environmental problems due to the persistence of pollutants and their carcinogenic and mutagenic compounds, which accumulate in soil, infiltrate into the groundwater and threaten human health and ecological security 1. In-situ soil flushing treatment where a water-based solution containing the surfactant (with other conceivable amendments) is injected into the subsurface, has appealed to various researchers [2-4] due to the high efficacy of removing the non-aqueous phase liquids. This study focuses on the synergy effect of the Sodium Dodecyl Sulfate (SDS) surfactant, a polymer (Xanthan Gum), and silica nanoparticles on the removal of asphaltenic crude oil from saturated media. The formulation of chemical solution was optimized through the measurement of interfacial tension (IFT) between the crude oil

and aqueous phase, and emulsification studies. The stability of proposed nanofluid was evaluated using the measured zeta ( $\zeta$ ) potential values. The efficiency and pollutants removal mechanisms of optimized nano-enhanced chemical solution in porous media were assessed using a microfluidic device with heterogeneous pore and throat structure. The results showed that the values of IFT between the crude oil and aqueous phase decline in presence of SDS surfactant, and in the existence of silica nanoparticles the reduction is more dominant. The synergy of SDS-Xanthan Gum-silica nanoparticles resulted in better emulsification for asphaltenic crude oil and as a consequence more contaminates removal. The results of pore-scale investigation indicated that during in-situ surfactant flushing, the petroleum contaminants removal from porous media occurs mainly due to the mobilization and solubilization mechanisms. However, emulsification may also happen and contribute to the pollutants' removal. This study shows promising results for the application of the nano-enhanced chemical solution to improve the in-situ petroleum contaminants treatment.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## Pore-Scale Simulation of Mucilage Drainage in the Rhizosphere

**Author:** Omid Esmaelipoor Jahromi<sup>1</sup>

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Compared to bulk soil, the rhizosphere has different properties because of the existence of root mucilage which affects the physical, chemical, and also microbial processes. Hydraulic phenomena like limiting water flow at certain dry soil conditions, modulating extreme water contents by slow response to water potential changes; and also influencing solute transport and gas diffusion by varying the connectivity of liquid and gas phases are all classified under the set of the physical processes which are affected by mucilage in the rhizosphere.

Overview of the literature and previous models shows the lack of a three-dimensional pore-scale dynamic model for a better understanding of the connectivity between different phases during imbibition and drainage processes. A major challenge is that mucilage shows a complex behavior which at low concentrations is more like a liquid while at higher concentration when it is almost dry, it becomes a solid. In between, a viscoelastic state is observed and then, mucilage can be considered as a hydrogel.

In particular, this study will use the Lattice Boltzmann method as a powerful tool for fluid dynamics studies and the Discrete Element method for describing solids to present a three-dimensional pore-scale model to simulate the drainage of mucilage between two soil particles. The model will be examined by comparing simulation results and ESEM images of real systems. In real systems, due to the concentration of mucilage and the distance between soil particles, different structures

may be formed such as thin filaments or hollow cylinders. This model is able to reproduce observed structures, successfully.

The proposed model may provide us with a new perspective on hydrodynamic processes within the pore space in the rhizosphere. In addition, some other valuable data such as liquid bridges, connectivity of phases, solute transport and etc. would be resulted out of this model.

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MS9 / 356

## **Pore-by-pore modeling, calibration, and prediction of two-phase flow in mixed-wet rocks**

**Authors:** Sajjad Foroughi<sup>1</sup> ; Branko Bijeljic<sup>2</sup> ; Qingyang Lin<sup>3</sup> ; Ali Qaseminejad Raeini<sup>4</sup> ; Martin Blunt<sup>3</sup>

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In this study, a pore-network model as an upscaled representation of the pore space and fluid displacement is used to simulate and predict two-phase flow through porous media. The results of micro-CT pore-scale imaging experiments are used to calibrate the model, and specifically to find the pore-scale distribution of wettability. As wettability is an uncertain parameter in two-phase flow modeling, we employ energy balance to estimate an average, thermodynamic, contact angle in the model. This thermodynamic contact angle is used as the initial estimate of wettability. We then adjust the contact angle of each pore to match the observed fluid configurations in the experiment at the pore level as a nonlinear inverse problem. The proposed algorithm is implemented on two sets of steady-state micro-computed-tomography experiments for water-wet and mixed-wet Bentheimer sandstone. As a result of the optimization, the pore-by-pore error of fluid distribution between the model and experiment is decreased to less than that observed between repeat experiments on the same rock sample. After calibration and matching, the model predictions for upscaled parameters of capillary pressure and relative permeability are in good agreement with the experiments. The proposed algorithm leads to a distribution of contact angles around the thermodynamic contact angle. We show that the contact angle is spatially correlated over around 4 pore lengths, while larger pores tend to be more oil-wet. Using randomly assigned distributions of optimized contact angles in the model results in poor predictions of relative permeability and capillary pressure, particularly for the mixed-wet case. Also, analyzing the spatial correlation show a stronger for mixed-wet Bentheimer sandstone.

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MS11 / 230

## Pore-level observation of the transitional pore clogging by asphaltene deposition using micromodels

**Author:** Yutaka Onaka<sup>1</sup>

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Asphaltene is defined as the crude oil component, which is soluble in toluene and insoluble in light-n-alkane [1,2]. In the development of oil fields, the deposition of precipitated asphaltene in a reservoir is a serious problem since it leads to clogging of the pores of the rock, resulting in a reduction in permeability [3]. Wang & Civan's model, which was constructed based on DBF (deep-bed-filtration) theory, has been commonly used in Darcy-scale simulations to calculate the volume of asphaltene deposition [4,5]. In this model, the deposition rate of asphaltene is expressed by the summation of three terms: surface deposition caused by adsorption or gravity sedimentation, entrainment, and clogging of pores. Each term contains an empirical coefficient that needs to be tuned by comparing the experimentally measured permeability and the calculated one [6], which means that these coefficients cannot be determined without experiment. Pore-scale observation of the deposited asphaltene can directly evaluate the types of deposition. The observation using X-ray microtomography showed that the cluster of deposited asphaltene clogged multiple pores after flooding with crude oil, which contains asphaltene, into a rock [7]. Although this shows the actual behaviour of the deposition, the transition of the clogging is still unknown. Several studies have been conducted with microfluidics experiments to capture the transient flow inside a transparent chip by a microscope. The process from precipitation to deposition of asphaltene at the wall of the chip [8] or dissolving behaviour of the asphaltene [9] have been visualised. However, the deposition process to clog the pores and the contribution of each type of deposition to the clogging is not well investigated.

In this study, the transition of asphaltene deposition inside porous media was visualised by a glass-made micromodel. In the micromodel, a lattice-like pore-network area with 6 cm in length and 1 cm in width was chemically etched. Each pore size was 100  $\mu\text{m}$  in width and 110  $\mu\text{m}$  in depth. Crude oil was mixed with n-heptane as a precipitant of the asphaltene and injected into the micromodel at a rate of 0.7 ml/h, which was equivalent to a Darcy velocity of  $1.94 \times 10^{-4}$  m/s. During the injection, the area composed of 2.5 mm length and 1.8 mm width was monitored with a microscope with a ten magnification lens to obtain two-dimensional sequential images. Image analysis was conducted to identify deposited asphaltene.

We observed transitional processes from the deposition of asphaltene particles to the clogging of the pore spaces. At the initial stage, the deposition occurred at the local site of the pores. The deposited site grew by the accumulation. Finally, these local clusters were connected, resulting in the complete clogging of the area. The area of occupancy of the pores clogged with asphaltene linearly increased to 57.6%.

The ratio of deposition type to total deposition area was evaluated quantitatively to investigate each type's contribution to the permeability reduction.

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MS1 / 131

## Pore-scale Investigation of the Capillary Pressure Effect on the Upward Migration of Hydrogen through Water-filled Porous Media

**Author:** Mehrdad Vasheghani Farahani<sup>1</sup>

**Co-authors:** Aliakbar Hassanpouryouzband<sup>2</sup>; Katriona Edlmann<sup>2</sup>

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An efficient energy-management strategy is critical for the fast transition of the global energy sector towards operation with 100% renewable or low-carbon energy, of which energy-storage is a key part. Among energy storage technologies, the geological storage of hydrogen, utilising excess or curtailed renewable energy and electrolysis has emerged as a Terawatt-scale, clean and sustainable energy storage technology. As such, understanding the complex flow behaviour of hydrogen in these storage reservoirs is critical. In this study, we explored how hydrogen with a lower density than water migrates through water-filled porous media, aiming at characterising the interplay of the gravity and capillary forces. Two dimensional multicomponent-multiphase (MCMP) lattice Boltzmann (LB) simulations were conducted using the Shan-Chen pseudo-potential model with a D2Q9 configuration. The model was firstly validated by conducting a numerical simulation for Poiseuille flow and comparing the simulation results against the analytical solution and performing a MCMP simulation for capillary rise phenomenon in a capillary tube. The validated model was then used to simulate the upward (y-direction) migration of a hydrogen plume with an initial saturation ( $Sh,i$ ) of 10% in a porous column, partially filled with water ( $Sw,i = 90\%$ ). The porous column is homogeneous, consisting of equally sized grains ( $r$ ), placed with a simple cubic packing configuration. Periodic boundary conditions were considered at the right and left borders of the column and a half-way bounce-back boundary condition was assumed for all solid boundary conditions as well as the boundaries at the top and bottom. The effect of the capillary pressure on the upward migration of hydrogen was captured by: (i) running the LB simulation at different “ $r$ ” values while keeping the porosity at a typical cubic packing constant value ( $\sim 40\%$ ), (ii) obtaining the ultimate saturation ( $Sh,u$ ) of accumulated hydrogen at the 10% upper region of the porous medium at the equilibrium conditions, and (iii) comparing  $Sh,u$  with  $Sh,i$ . The simulation results confirm that the structure of mesoporous media control, the dynamics of gravitationally unstable flow and the capillarity have a major contribution to the flow behaviour of hydrogen. Ultimately, the results have implications for accurate projection of the hydrogen plume evolution and as such the design of various storage options and well production strategies.

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MS21 / 733

**Pore-scale Mixing and the Evolution of Hydrodynamic Dispersion****Authors:** Marco Dentz<sup>1</sup> ; Alexandre Puyguiraud<sup>2</sup> ; Philippe Gouze<sup>3</sup><sup>1</sup> IDAEA-CSIC<sup>2</sup> IDAEA - CSIC<sup>3</sup> Geoscience Montpellier, CNRS, Université de Montpellier**Corresponding Authors:** philippe.gouze@umontpellier.fr, marco.dentz@csic.es, alexandre.puyguiraud@gmail.com

Transport of dissolved substances through natural and engineered porous media is determined by the inherent complexity of the pore space, and diffusive mass transfer within and between pores. The interplay of pore-scale mixing and network-scale flow variability are key for the understanding of transport and contact processes in porous media with diverse applications ranging from groundwater contamination and geological carbon dioxide storage, to the design of batteries, and transport in brain microcirculation. Therefore, hydrodynamic transport has been the focus of research over decades in different disciplines. Nevertheless, questions of fundamental nature remain concerning both the evolution of hydrodynamic dispersion, and the dependence of asymptotic hydrodynamic dispersion coefficients on the Péclet number. We use a Lagrangian framework to identify and quantify three fundamental mechanisms of pore-scale mixing that determine the stochastic dynamics of pore- and network-scale particle motion: (i) The smoothing of intra-pore velocity contrasts, (ii) the increase of the tortuosity of particle paths, and (iii) the setting of a maximum time for particle transitions. Based on these mechanisms, we derive an upscaled approach that predicts anomalous and normal hydrodynamic dispersion in terms of the characteristic pore length, Eulerian velocity distribution and Péclet number. The theoretical developments are supported and validated by direct numerical flow and transport simulations in three-dimensional digitized porous medium samples. Solute breakthrough curves are characterized by intermediate power-law behaviors and exponential cut-off, which reflect pore-scale velocity variability and intra-pore solute mixing. Similarly, dispersion coefficients evolve from molecular diffusion at early times to asymptotic hydrodynamic dispersion via an intermediate superdiffusive regime. The theory captures the full evolution from anomalous to normal transport behavior at different Péclet numbers as well as the Péclet-dependence of asymptotic dispersion.

It is not constrained by transport measurements. The fundamental nature of the considered flow and transport processes allows application of the key elements of the derived theory to transport of dissolved chemicals, bacteria and colloids in a wide range of porous media also under different flow conditions.

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## Pore-scale analysis of gas injection in gas-condensate reservoirs

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Production from gas condensate reservoirs can be significantly improved with gas injection. Several approaches to the method have been proposed in the literature, aiming pressure maintenance in the reservoir and/or re-evaporation of the deposited condensate, with promising results. However, the effects of complex phase behavior arisen from the interaction between injected gas and accumulated fluids in the porous medium are often overlooked. Local changes in composition can alter significantly both bulk and interfacial properties of gas and liquid phases, affecting, therefore, their displacement in porous media. In order to investigate these effects at the micro-scale, we used a compositional pore-network model to reproduce gas injection into porous media after condensate accumulation. The flow of a representative gas-condensate fluid through a sandstone-based network at different depletion levels was followed by the injection of CO<sub>2</sub>, N<sub>2</sub>, CH<sub>4</sub> and C<sub>2</sub>H<sub>6</sub>, and the flow improvement was evaluated. Final saturations, relative permeabilities and recovery of heavy hydrocarbon components were quantified to compare the efficacy of each injection scenario. Results indicated that CO<sub>2</sub> and C<sub>2</sub>H<sub>6</sub> had the greatest potential to re-evaporate condensate banking and restore flow capacity, among the tested gases. Contrarily, insufficient amounts of CH<sub>4</sub> and N<sub>2</sub> injection could even lead to flow impairment, due to the observed gain in liquid dropout and increased interfacial tension. Additionally, N<sub>2</sub> injection could not mobilize the heaviest condensate components in any tested scenario.

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## Pore-scale capillary heterogeneity in reservoir rocks and its influence on reservoir-scale flow

**Authors:** Zoe Shipton<sup>1</sup> ; Carla Romano<sup>1</sup> ; Charlotte Garing<sup>2</sup> ; James Minto<sup>1</sup> ; Sally Benson<sup>3</sup> ; Rebecca Lunn<sup>1</sup>

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It is increasingly important to understand multiphase fluid flow in rocks: not just in conventional hydrocarbon applications, but in geoenvironmental technologies for net zero such as geothermal heat production, carbon capture and storage, subsurface storage of energy fluids etc. Deformation bands in sandstone reservoir rocks are localized zones of grain crushing, grain reorganisation and/or cementing that can form capillary barriers to fluid flow, and which are common in. Here we analyse the extent and mechanisms of fluid compartmentalization due to clustered deformation bands. Multiphase fluid flow experiments were performed on a core sample of Navajo sandstone that contained fine-scale laminae cut by diversely oriented clusters of deformation bands. Medical X-ray CT images were acquired while nitrogen was injected at progressively higher flow rates into a water-saturated core during transient and steady-state conditions. Spatial and temporal analyses of the non-wetting phase plume migration suggest that the deformation bands act as capillary barriers, resulting in the

development of an extremely tortuous saturation front. Differential pressure behavior across the core is linked to breakthrough of N<sub>2</sub> into the individual compartments, resulting in highly variable N<sub>2</sub> saturation throughout the experiment. Migration into downstream compartments occurs when capillary entry pressure is exceeded across restricted portions of the bands. These observations confirm that clusters of deformation bands have the potential to strongly compartmentalize a subsurface reservoir, increasing the risk of overestimating reservoir capacity, and requiring novel production strategies to minimize the effect.

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MS6-B / 567

## Pore-scale effects during the transition from capillary- to viscosity-dominated flow dynamics within microfluidic porous-like domains

**Authors:** Andreas Yiotis<sup>None</sup>; Nikolaos Karadimitriou<sup>1</sup>; Ioannis Zarikos<sup>2</sup>; Holger Steeb<sup>3</sup>

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In this work, numerical and physical experiments were carried out involving two-phase flow in an artificial, transparent porous medium, namely a micromodel. The pore structure was formed by the combination of disordered pillar-like obstacles. With the use of high sensitivity pressure sensor at the flow inlet we were able to monitor the pressure fluctuations under fixed flux boundary conditions. We were able to capture the dynamics of the advancing interface in terms of pressure, and at the same time capture the corresponding phase distribution with optical microscopy. The experimental part of this work covered 4 orders of magnitude in terms of capillary number, as the means to depict the transition of the flow regime from a capillarity- to a viscosity-dominated one. Phenomena like Haines jumps and sequentially pore filling and simultaneous pore filling were visualized with respect to each flow regime. For the capillarity-dominated regime we were able to recover a clear correlation between the boundary pressure readout and the corresponding throat size of the invasion pressure based on Young-Laplace equation. This correlation gradually faded away, of course, as the system would transition to a viscous flow regime. A robust Level-Set model was able to be validated experimentally by explicitly tracking the interfacial dynamic at a sub-pore scale resolution under identical flow and pore structure conditions. The numerical model was validated against well-established theoretical models which account for both effects, capillarity, and viscosity, on interfacial dynamics. The proposed numerical model recovers very well the experimentally observed flow dynamics, both in terms of phase distribution patterns and inlet pressures, but also the effects of viscous flow on the apparent (i.e. dynamic) contact angles in the vicinity of the pore walls.

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## **Pore-scale hydro-mechanical modeling of gas transport in coal matrix**

**Authors:** Ahmad Mostafa<sup>1</sup> ; Luc Scholtès<sup>2</sup> ; Fabrice Golfier<sup>1</sup><sup>1</sup> *Université de Lorraine, CNRS, GeoRessources, 54000 Nancy, France*<sup>2</sup> *Université Clermont Auvergne, CNRS, IRD, OPGC, Laboratoire Magmas et Volcans***Corresponding Authors:** fabrice.golfier@univ-lorraine.fr, luc.scholtes@uca.fr, ahmad.mostafa@univ-lorraine.fr

Coal beds are dual permeability systems characterized by a porous matrix enclosed within sets of orthogonal fractures known as cleats. Production of coalbed methane (CBM) consists of desorbing methane from the low permeable coal matrix to the high permeable cleat system. Unlike in conventional reservoir exploitation, sorption mechanisms cause shrinkage and swelling of the matrix which increases the complexity of the phenomena at stake, leading to complex reservoir behaviors in terms of production.

A 3D discrete element method (DEM) coupled to a pore-scale finite volume method (PFVM) is used here to better understand the different mechanisms at stake. The model, implemented in the open-source software Yade Open DEM (Smilauer et al., 2015), is an offspring of the hydro-mechanical model proposed by Catalano et al. (2014). The coal matrix is treated as an assembly of bonded particles interacting one with another through elastic-brittle contact laws. The pore space is discretized into tetrahedra, generated from a regular triangulation of the particle assembly. Both Knudsen and surface diffusions, as well as sorption processes, are modeled considering the coal matrix as a microporous material. The method is hydro-mechanically coupled in the sense that changes in pore pressure produce hydrostatic forces that deform the solid skeleton, while deformation of the pore space induces pore pressure changes that promote interporal flow. Besides, sorption induced deformations are taken into account by considering an additional pressure term related to the concentration of gas within the medium (the so-called solvation pressure).

In this work, we first present the model and its constitutive equations. We assess its capabilities by comparing its predictions to well-established solutions describing diffusive flow in porous media as well as to classic poroelasticity concepts. In particular, we focus on the influence of sorption induced deformations on the Biot coefficient estimation. Finally, we compare the model predictions to swelling test data from the literature to illustrate its consistency.

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

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## Pore-scale imaging of unsaturated solute transport to determine the influence of fluid distribution on solute spreading and mixing

**Authors:** Stefanie Van Offenwert<sup>1</sup> ; Veerle Cnudde<sup>1</sup> ; Shan Wang<sup>1</sup> ; Tom Bultreys<sup>1</sup>

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Solute transport in unsaturated porous media is a key process for various applications, such as groundwater flow and building stone performance. The distribution of the immiscible fluids controls which parts of the pore space are accessible for solute transport. This may lead to a bimodal velocity distribution in the solvent phase with stagnant and flowing regions (Jiménez-Martínez et al., 2017), characterized by non-Fickian solute transport. Hasan et al. (2019) showed that there are still fundamental inconsistencies between different modelling approaches, spurring the need for experimental validation. However, due to methodological challenges there are only few experimental studies that target unsaturated solute transport in rocks at the pore scale (Hasan et al., 2020).

In this study, we visualized the spreading of a solute through partially water-saturated sintered glass and Bentheimer sandstone samples. After a drainage and imbibition cycle with water and n-decane, leaving a significant amount of the latter trapped in the pore space, an aqueous tracer solution (10 wt% KI) was injected with a constant flow rate. Transient pore-scale concentration fields in the sample were imaged in 3D by using fast laboratory-based X-ray micro-CT (time resolution of 15 s, voxel size of 13 µm). To determine the influence of the non-wetting phase on the solute transport, single-phase experiments were also performed on the same samples. By extracting a pore network and performing a pore-scale image analysis work flow (Van Offenwert et al., 2019) we investigated the existence of stagnant and flowing regions. Furthermore, we studied the influence of the fluid phase distribution on solute mixing and spreading. These results can improve our understanding of non-Fickian solute transport. Our novel methodology can also be used to validate two-phase solute transport simulations in rock types with different pore-scale heterogeneity.

### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

Hasan, S., Joekar-Niasar, V., Karadimitriou, N. K., & Sahimi, M. (2019). Saturation-Dependence of Non-Fickian Transport in Porous Media. *Water Resources Research*. <https://doi.org/10.1029/2018WR023554>

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MS1 / 104

## Pore-scale modelling and sensitivity analyses of hydrogen-brine multiphase flow in geological porous media

**Authors:** Leila Hashemi<sup>1</sup> ; Martin J. Blunt<sup>2</sup> ; Hadi Hajibeygi<sup>1</sup>

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Supply of green energy to society can successfully happen if large-scale storage technologies are developed. Underground hydrogen storage (UHS) in initially brine-saturated deep porous rocks is a promising option, due to hydrogen's high specific energy capacity and the high volumetric capacity of aquifers.

Appropriate selection of a feasible and safe storage site vitally depends on understanding hydrogen transport characteristics in the subsurface. Unfortunately there exist no robust experimental analyses in the literature to properly characterise this complex process. As such, in this work, we present a systematic pore-scale modelling study to quantify the crucial reservoir-scale functions of relative permeability and capillary pressure and their dependencies on fluid and reservoir rock conditions. To conduct a conclusive study, in the absence of sufficient experimental data, a rigorous sensitivity analysis has been performed to quantify the impacts of uncertain fluid and rock properties on these upscaled functions. The parameters are varied around a base-case, which is obtained through matching to the existing experimental study. Moreover, cyclic hysteretic multiphase flow is also studied, which is a relevant aspect for cyclic hydrogen-brine energy storage projects. The present study applies pore-scale analysis to predict the flow of hydrogen in storage formations, and to quantify the sensitivity to the micro-scale characteristics of contact angle (i.e., wettability) and porous rock structure.

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MS9 / 623

## **Pore-scale observation and insight on how wettability impacts oil recovery and its dependence on rock structure**

**Authors:** Fanli Liu<sup>1</sup> ; Moran Wang<sup>1</sup>

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The wetting condition of the reservoir is known to have a big impact on oil recovery by waterflooding and wettability alteration has been widely accepted as one major mechanism of many enhanced oil recovery techniques. However, it remains not fully clear what wetting conditions lead to the maximum oil recovery, and there were seemingly contradictions between different studies in terms of the optimal wettability. Although several mechanisms were proposed to explain how wettability influences the waterflooding process, the relation between such influences and oil recovery can often be uncertain, and the mechanism themselves sometimes lack direct evidence.

This work looks directly into the pore-scale phenomena to add to the understanding of how wettability impacts the trapping and recovery of oil. First, fully capillary-dominated waterflooding processes are considered, as is the common assumption under reservoir condition. It is found that depending on the pore-scale geometry, either strongly water-wet or weakly water-wet can lead to the least trapping of oil, and relevant mechanisms are proposed based on the direct pore-scale observations. Then the assumption of capillary forces fully dominating at low capillary number is challenged as it is shown that the viscous force can have a big impact on the flow pattern and thus oil trapping, even at low capillary number and without viscous fingering. Finally, the relation between oil recovery and wettability is discussed and summarized based on the new findings, with emphasis on how rock structure can alter the relation.

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MS5 / 361

## Pore-scale origin of flow-induced bio-aggregation

**Author:** Sang Lee<sup>None</sup>

**Co-authors:** Eleonora Secchi<sup>1</sup>; Peter Kang<sup>2</sup>

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Microbes in natural and engineering systems are often found as aggregates consisting of microbial communities, organic and inorganic matters, and water. Such bio-aggregates play important roles in shaping biogeochemistry of soil and groundwater environments, clogging of porous media, biofilm formation, and human lung infections [1 – 3]. In addition, aggregated cells are reported to have enhanced protections against external stresses such as anti-biotics, nutrient starvation, oxidative stress, etc., helping microbes to cope with environmental changes [3]. Therefore, understanding how bio-aggregates are formed has been an active area of research in not only engineering and natural sciences but also in clinical and evolutionary standpoints. While bio-aggregates are widely generated in porous systems, the role of pore-scale flow and porous media structure on aggregation is still poorly understood. In this study, we combine microfluidics experiments and three-dimensional (3D) numerical simulations to demonstrate that the unique 3D flow structure at the constriction points of pore-throats, which is ubiquitous in porous media, induces bio-aggregate formation.

We use a single channel with a sinusoidal pore-throat as an analog for a porous system (FIG. 1A). Upon injection of an *E. coli* suspension (OD<sub>600</sub> = 0.1) at a constant flow rate (0.2 μl/min), we observed the formation of bio-aggregates at the pore-throat while in a straight channel only attachment and growth were detected (FIG. 1B - D). Pore clogging and pressure build-up occur as *E. coli* cells aggregate, which eventually lead to the detachment and flushing of bio-aggregates. A series of laboratory and numerical experiments revealed that 3D secondary flows facilitate attachment and capture of cells at the pore-throat, inducing aggregation. We further identified a critical shear stress value (~ 1.8 Pa) below which an aggregate forms and above which biofilm streamer-like morphology is found. Finally, we show that when the shear stress at the pore-throat is maintained below the critical shear stress, the pore-throat is rapidly clogged by bio-aggregates.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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Poster + / 546

# Pore-scale physics in imposed thermal gradient drying in porous media using Lattice Boltzmann Method

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**Co-authors:** Divyansh Pandey<sup>2</sup> ; Dasika Prabhat Sourya<sup>3</sup> ; Evangelos Tsotsas<sup>4</sup> ; Abdolreza Kharaghani<sup>5</sup> ; Vikranth Kumar Surasani<sup>6</sup>

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Drying of porous media sounds simple yet it is complicated to understand the physics behind it. As drying is an energy-intensive process, it is necessary to understand the trade-off between energy costs and efficient drying process using recently developed mathematical models. In our previous presentations 1–[3], we addressed a novel isothermal diffusion dominated drying model using the mesoscopic model: Lattice Boltzmann Method (LBM). It has emerged as a powerful modeling tool for multiphase flows in complex pore structures because of its easiness of implementing the no-slip boundary conditions with intricate solid surfaces. The complex pore-scale physics involving Haines Jumps and its implications to drying kinetics was presented. In this work, we are extending our previous works to include thermal drying model using imposed thermal gradients. A linearly varied stationary temperature profile is imposed along the depth of the porous medium. The preferential heating is of two types: positive thermal gradient where temperature varies from top to bottom in increments (e.g., Convective drying) and negative thermal gradient where the temperature varies in decrements (e.g., Contact heating mode of drying). According to the competition between capillary, viscous and gravitational forces, different kinds of invasion patterns are observed. The invasion-percolation (IP) of stabilizing and destabilizing drying fronts are discussed, where in the two sided (primary and secondary) drying regimes is observed. Thanks to the automatic interface capturing method which is inherently present in the multiphase Shan Chen LBM, it is exciting to observe capillary condensation in negatively imposed thermal gradient. In the past, condensation is implemented for partially filled throats[4]. However, for the first time, evaporation-condensation phenomena in drying of capillary porous media is completely addressed through LBM simulations[5]. Finally, the micro-macro interactions and the future of forming a freely evolving thermal drying model in LBM are elucidated.

## Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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## Pore-scale simulations of water droplet interaction with a hydrophobic wire screen for purpose of Water-Diesel separation

**Authors:** Omar Elsayed<sup>1</sup> ; Ralf Kirsch<sup>2</sup> ; Sebastian Osterroth<sup>2</sup> ; Sergiy Antonyuk<sup>3</sup>

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The new constraints for reducing hazardous emissions and sustainable fuel production led to an increased usage of ultra-low-sulfur diesel (ULSD) and bio-diesel. Such fuels have a significantly lower surface tension coefficient in comparison to Diesel. Consequently, the design of separators in diesel fuel filters meeting today's performance requirements imposes a challenge to the developing engineer and for suitable simulation techniques. The challenge in modeling and simulation of such systems is that different parameters of the microscale control the overall performance of water-diesel separators. On the microscale, the fiber radius is considered as the dominant length scale. Droplet sizes and shapes should be resolved for accurate computation of the pressure and velocity fields. A sequence of successive coalescence on the microscale leads to the formation of large droplets, which fall down through the gravitational force. This transport is known as drainage. In the case of high adhesive force, the droplets do not fall down. Large droplets that do not have enough gravitational force are ruptured and the overall pressure drop increases significantly.

The presentation is devoted to the modeling and simulation of the interaction between the water droplets and the separator screen taking into account different parameters: geometric properties of the mesh, contact angle, surface tension coefficient, inflow velocity, and droplet radius. First, we quantify the shape of the droplet in different flow scenarios. Secondly, we fit the drag coefficient and the overall pressure drop for a single water droplet partially clogging a wire mesh based on the shape of the droplet. We also quantify the maximum pressure drop at which rupture of droplets occurs. Finally, we quantify the largest droplet that can be held by a mesh before drainage occurs and its corresponding drainage velocity. The simulations are carried out using the finite volume computational fluid dynamics library OpenFOAM®. We use a new scheme for the accurate computation of surface tension force 1.

These results help to develop a simplified description of the dynamics of water droplets interacting with a mesh screen. Applying a proper mathematical averaging technique will lead to an averaged description of the collective dynamics and building a macroscopic model that is capable of estimating the performance of the Water-Diesel separator in a specific application.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

O. Elsayed., S. Antonyuk., R. Kirsch., and S. Osterroth., "Computer-aided study of the Diesel-water separation efficiency of screen meshes," in *FilTech*, 2019. **Acceptance of Terms and Conditions:**

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MS9 / 510

## Pore-scale study to understand the influence of porosity on mass transport in Anodic Porous Transport Layer of PEM electrolyser



## using Lattice Boltzmann Method

**Authors:** Shubhani Paliwal<sup>1</sup> ; Supriya Bhaskaran<sup>None</sup>

**Co-authors:** Jenil Agarwal<sup>2</sup> ; DEBASHIS PANDA ; Nicole Vorhauer<sup>3</sup> ; Tanja Vidakovic-Koch<sup>4</sup> ; Evangelos Tsotsas<sup>5</sup> ; Vikranth Kumar Surasani<sup>6</sup>

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The surging demand for energy and the environmental impacts of conventional sources such as fossil fuels are the ground for the upcoming predicted energy crisis. Electrolysis of water has emerged as a promising technology for surplus production and storage of pure hydrogen as an alternative green fuel. Polymer Electrolyte Membrane (PEM) water electrolyzers are used for the on-demand power generation without any greenhouse gas emissions. The anodic Porous Transport Layer (PTL) of PEM electrolyzers serves channels for water to reach the active sites of the catalyst layer as well as escape pathways for oxygen. The material properties of the anodic PTL such as porosity, pore size distribution, fibre thickness and tortuosity play a major role in the performance of the PEM electrolyzers. Anodic PTL has a fibrous porous structure in which pore volume is larger than the throat volume. This results in oxygen bubble snap-off and fast finger generation according to the local porosity variation in the PTL which ultimately affects the efficiency of the oxygen removal process. However, this cannot be studied using well-established Pore Network Modelling (PNM) as in the reconstruction step, the pore volume is regarded as smaller than the pore volume. On the other hand, mesoscale models such as Lattice Boltzmann Model (LBM) 1 has emerged as a promising technique for simulating such fluid transport and flows in porous media [2]. In this study, a multicomponent Shan Chen LBM is implemented to study the evolution of oxygen-water phase distribution in 3D anodic PTL of the electrolyser. The PTL features such as porosity and pore size distribution are studied for the minimization of oxygen saturation. The porosity of the PTL can be varied by the thickness of the fibres and the number of the fibres. The influence of these two parameters at the same porosity of the PTL is studied in detail which further affects the performance of the electrolyser. Moreover, bubble snap-off, bubble coalescence, and slug flow of oxygen finger are discussed in a three-dimensional fibrous anodic PTL. This work is a fundamental step to understand the morphology of the anodic PTL to enhance the rate of oxygen removal by rapid bubble coalescence and water delivery to the active sites of the catalyst layer.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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## Pore-throat structure and fractal characteristics of shale oil reservoirs in the Lucaogou Formation of Jimusaer Depression, China

**Authors:** Rui Shen<sup>None</sup> ; Xiaoyi Zhang<sup>None</sup> ; Wei Xiong<sup>None</sup> ; Hekun Guo<sup>None</sup> ; Hongtao Zhou<sup>None</sup> ; Hang Yang<sup>None</sup> ; Huichen Ren<sup>None</sup>

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The shale oil reservoir of the Lucaogou Formation in Jimusaer Depression, Xinjiang Province, China, features a structure exhibiting several issues, such as complex lithology, and an ambiguous pore-throat structure and configuration. To resolve these issues, numerous contemporary experimental methods, including focused ion beam scanning electron microscopy (FIB-SEM), nano-scale CT scanning (Nano-CT), atomic force microscopy (AFM), and low-temperature N<sub>2</sub> adsorption (LTNA) have been utilized, to study the pore-throat structure and the full-scale pore size distribution. Among these techniques, FIB-SEM and Nano-CT have been widely employed to examine the distribution, configuration, and connectivity of the pores and throats that belong to the diameter range of 7 nm–1 μm and greater than 1 μm, respectively. Using these two scanning techniques, the full-scale pore-throat size distribution curves determining the relationship between the pores throat volume of unit sample weight have been plotted. The results implied by these curves in combination with the results of the AFM and LTNA curve hysteresis loop facilitate the comprehensive analysis of the pore-throat characteristics of various lithological samples, including properties such as fractal dimension, pore morphology, and pore structure. It can be deduced from the results obtained that the shale oil reservoir located in the Jimusaer Depression embodies source rocks that are rich in organic matter, however, the porosity level of these rocks remains low, which makes it befitting only as a storage space, while the siltstone and dolarenite exhibit larger pores and throats, maintaining good connectivity. The pores found in the siltstone rocks of this reservoir are predominantly plate or wedge-shaped, and dolarenite pores mostly take cylindrical-like or elliptic cylinder shapes with one or two open ends. The fractal dimension of the pores in siltstone and dolarenite is usually less than 2.75, while the specific surface area remains less than 8 m<sup>2</sup>/g. Siltstone and dolarenite rocks not only form the reservoir space, but also function as the chief percolation channels.

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## **Poromechanics in extremely large deformation: swelling and fracture**

**Author:** Jacques Huyghe<sup>1</sup>

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Biomedical engineers face porous media with very low stiffness, high osmolarity and extremely large deformations. Examples are superabsorbent hydrogels and living cells. Volume strains above 1000 % strain are commonplace in diapers, female pads and growth plates. The strong nonlinearities of large deformation formulations of poromechanics hamper the use of analytical solutions. Large deformation u-p formulations fail in this regime. This means that simulation tools of poromechanics are inapt to a great deal of biology, which typically unfolds in the intracellular space. Local mass balance violation is the culprit under extremely large deformations. In order to address this issue, we developed a mixed hybrid formulation of poromechanics of swelling gel based on a Raviart-Thomas finite element. This formulation strictly complies with local mass balance. Swelling computations are possible down to a shear modulus of 10 kPa. Surface instabilities easily develop as osmotic forces overtake the stabilising effect of the elasticity. Fracture simulation using large deformation XFEM including flow within the crack, between the crack and the formation and within the crack, allows for initiation, coalescence and bifurcation of cracks. XFEM computations predict experimentally observed staccato propagation of cracks in hydrogels. Constitutive modelling of swelling require

the concurrent use of elastic, mixing and ionic energies in Flory-Rehner swelling model. Interaction terms between elastic and ionic energies occur because the stiffness of gels directly depends on ionic concentrations. Future perspectives on constitutive modelling of swelling and fracturing gels include herniation of intervertebral disc, mechanotransduction of extracellular matrix and design of biomimetic hydrogels. Hydraulic fracturing of shale is an important geotechnical application.

The presented work is collaboration with Cong Yu (Eindhoven University of Technology), Jingqian Ding (Eindhoven University of Technology), and Eanna Fennel (University of Limerick.)

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## Porosity Dynamics through Carbonate-Reaction Kinetics in High-Temperature Aquifer Storage Applications

**Author:** Burt Tilley<sup>1</sup>

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While near-surface geothermal energy applications for the heating and cooling of buildings have been in use for decades, their practical adoption is limited by the energy transport rates through soils. Aquifers provide a means to use convective heat transport to improve heat transfer between the building and the aquifer. However, the solid matrix in the aquifer is carbonaceous in nature, and calcification prevention techniques in the heat exchangers for the building also lead to dissolution of the aquifer matrix. Due to the Arrhenius nature of the reaction, dissolution rates may decrease with increasing temperature. An effective medium model is derived for the energy, calcium species, and fluid transport through a dynamic calcite porous medium which undergoes a reaction between the matrix and fluid. To better discern how these competing phenomena affect thermal transport in the aquifer, a two-dimensional Cartesian system is considered, where the vertical axis is parallel to the borehole axis, and flow is in the horizontal direction. An effective medium model is derived for the energy, calcium species, and fluid transport through a dynamic calcite porous medium which undergoes a reaction between the matrix and fluid. Since the fluid velocity decays algebraically with radial distance from the borehole axis, two flow regimes are considered. One regime, far from the borehole where flow rates are small, conductive thermal transport acts faster than the species transport, leading to a case where precipitation dominates and regions of the smallest porosity contract to limit energy recovery. In regions with larger porosity, moderate advection of the species is sufficient to prevent significant pore closures over the time scale of exploration. The second regime, closer to the borehole, larger flow rates reduce species concentrations sufficiently to dissolve the solid phase between pores. In this second regime, Taylor dispersion effects in both energy and species transport compete, but thermal conduction acts more slowly than advection, promoting dissolution. The critical limitation in modeling the long-term evolution of the aquifer structure is the in situ dissolution rate.

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## Porosity-permeability relationships for subflorescent salt crusts from evaporation of sand columns with varying initial salt concentration

**Authors:** Joseph Piotrowski<sup>1</sup> ; Dongwon Lee<sup>2</sup> ; Andreas Pohlmeier<sup>3</sup> ; Harry Vereecken<sup>None</sup> ; Holger Steeb<sup>4</sup> ; Johan Alexander Huisman<sup>None</sup>

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Salt precipitation due to evaporation from porous media leads to the formation of a salt crust that affects the flow and transport of water and solutes in the top layer of a porous medium, and causes amongst others soil salinization, erosion and land loss, as well as damage to building materials. Despite extensive research on evaporation of saline solutions from porous media, little is known about the effective transport properties of evolving salt crusts besides their importance for accurate modeling of evaporation. Most REV-scale models use porosity-permeability relations to describe how the reduction in porosity through salt precipitation affects the intrinsic permeability and thus the evaporation flux. The aim of this study was to experimentally investigate the relationship between porosity and intrinsic permeability of salt crusts and the associated evaporation using experiments with systematic variation of the initial salt concentration. For this, sand columns were prepared with solutions of  $\text{MgSO}_4$  at 0.32 mol/L, 0.64 mol/L, and 0.96 mol/L initial concentration and evaporated until 40%, 30%, or 20% final saturation within the corresponding sample was reached. The mass loss of every sample was measured once a day using a balance in order to determine the evaporation rate. The intrinsic crust permeability was determined using gas flow through the separated dried salt crusts. Additionally, nine selected crusts were partly scanned with a micro-XRCT set-up with 4  $\mu\text{m}$  resolution per voxel in order to determine porosity. The results showed that the evaporation rate was higher for the samples with lower initial concentration, which was attributed to the higher initial saturation pressure and the slower concentration increase of the solution during evaporation. It also was found that the permeability decreased with decreasing final saturation (i.e. increasing time of evaporation) and with increasing initial concentration. This is attributed to the varying amounts of precipitated salt that reduced the pore space. The XRCT measurements showed that subflorescent salt precipitation resulted in deformation of the unconsolidated sand. After segmenting the XRCT grey-scale data sets into air, sand and salt phases using k-means clustering, the segmented sand fraction ranged from 0.35 and 0.49, which was lower than the sand fraction of the initial sample (0.62). This observed deformation is in conflict with the common assumption in modeling evaporation of saline solution with subflorescent salt precipitation, where the porous matrix is assumed to be rigid. Despite the observed deformation, it was found that the initial void fraction (0.38) was reduced to void fractions between 0.12 and 0.31. In addition, a significant correlation between porosity (void fraction) and intrinsic permeability was obtained. However, the use of this porosity-permeability relation in REV-scale modelling of evaporation is not recommended as the change of the pore space not only depends on the precipitated salt volume but also on the (volumetrical) deformation of the porous matrix.

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Poster + / 743

## Porous Media Flow as a Heat Sink in a Triple Layered Electromagnetic Heat Exchanger

**Author:** Ajit Mohekar<sup>None</sup>

**Co-authors:** Burt Tilley<sup>1</sup>; Vadim Yakovlev<sup>1</sup>

<sup>1</sup> *Worcester Polytechnic Institute*

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An electromagnetic (EM) heat exchanger (HX) converts EM energy into heat or useful mechanical work. Examples of EM HXs are microwave thermal thrusters where high-power microwave heating is utilized to produce thrust from compressed gases, solar-thermal panels where a fluid is heated through solar radiations, etc. Our research is focused on modeling an EM HX useful in wireless power beaming application where energy is transmitted in the form of EM waves through the atmosphere and the HX acts as a receiver end. The structure of such an EM HX includes a lossy ceramic material, which is heated by EM waves, and bounded on two sides by a rigid porous media, with perfect thermal contact between it and the lossy ceramic. A nonlinear phenomenon associated with EM processing of ceramic materials (without fluid flow), such as zirconia and alumina, is thermal runaway, where a small increase in incident EM power causes significant rise of ceramic temperatures (e.g., about 2000K for alumina). It is of interest to investigate if the phenomenon of thermal runaway can be utilized for efficient energy transfer between fluid and the ceramic along with safer operating temperatures.

We focus on modeling of this triple-layer porous-media-based EM HX subject to a pressure driven fluid flow through the porous regions. Plane EM waves are incident symmetrically on the structure; only the ceramic is heated by EM waves, and fluid in porous structure heats up due to thermal contact with the ceramic. We are motivated to investigate the problem because improved heat transfer between the ceramic and the fluid due to porous channels may lead to higher thermal efficiency of the power transfer, and the thermal runaway characteristics may be altered.

We consider Darcy flow of an incompressible fluid through porous channels and find that thermal efficiencies (based on thermal power delivered by the fluid) are low in the limit of low Péclet number. We then extend the model considering large Péclet numbers to include Taylor dispersion effects that are originated as a result of deviation of local microscopic velocity from the macroscopic Darcy-velocity. Since the axial heat-diffusion is expected to improve with Péclet number, we investigate how Taylor dispersion improves thermal efficiencies and affects the onset of thermal runaway in the ceramic. Temperatures during thermal runaway indicate that liquid coolants flowing through the porous channels rapidly change their phase into gases at STP. To better match experimental conditions, we consider compressible gases flowing through the porous channels, and incorporate work of thermal expansion done by the gases. Results from numerical model based on compressible Darcy flow in porous channels show that the work done by the gas can lead to Joule-Thompson cooling effect which then delays the onset of thermal runaway in the ceramic. Finally, we consider Forchheimer's correction to investigate how flow inertia affects the work of thermal expansion and Joule-Thompson cooling of the gas.

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MS21 / 342

## Positive feedback effects in 2D creeping flow of viscoelastic fluids through porous media amplify preferential flow paths

**Author:** Omar Mokhtari<sup>None</sup>

**Co-authors:** Yohan Davit<sup>1</sup> ; Michel Quintard<sup>1</sup>

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The flow of dilute polymer solution in model porous media consisting of an array of cylinder is considered. Numerical [1] and experimental [2] studies show that such flows are subject to the intensification of preferential flow paths. These pathways tend to favour shear stress and thus increase viscous dissipation and decrease permeability.

We seek to study the mechanisms of reinforcement of these preferential flow paths which are crucial to the understanding of these flows. We consider here the Oldroyd-B model of dilute polymer solutions.

The equations of the model are solved using a time prediction-correction scheme and MAC discretization in finite volume in space.

The flow around two cylinders in a channel is first studied. As experimentally observed in [3], preferential flows appear, depending on the gap between the cylinders.

We show that the reinforcement mechanism of the preferential flow paths is linked to the appearance of elastic membranes which will interact with the flow. Like gates, they will guide the flow to areas where the velocity is initially high.

We then show how this mechanism works in the flow through an array of cylinders and study its impact on the flow and its macroscopic properties.

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

[1] S. De, J.A.M Kuipers, E.A.J.F Peters, and J.T Padding. Viscoelastic flow simulations in random porous media. *Journal of Non-Newtonian Fluid Mechanics*, 248 :50–61, 2017.

[2] D.M. Walkama, N. Waisbord, and J.S. Guasto. Disorder suppresses chaos in viscoelastic flows. *Phys. Rev. Lett.*, 124 :164501, Apr 2020.

[3] C.C. Hopkins, S.J. Haward, and A.Q. Shen. Tristability in viscoelastic flow past side-by-side micro-cylinders. *Phys. Rev. Lett.*, 126 :054501, Feb 2021. **Acceptance of Terms and Conditions:**

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MS3 / 520

## Predicting the long-term thermal performance of EGS reservoirs from tracer tests using ensemble smoother with multiple data assimilation

**Authors:** Hui Wu<sup>1</sup> ; Pengcheng Fu<sup>1</sup> ; Adam Hawkins<sup>2</sup> ; Hwei Tang<sup>1</sup> ; Joseph Morris<sup>1</sup>

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The long-term heat extraction from enhanced geothermal systems (EGSs) highly depends on the flow and transport characteristics in the underlying fracture networks connecting injection and production wells. Tracer testing is a powerful diagnostic tool for subsurface fracture characterization. However, interpreting the obtained tracer data for long-term thermal performance prediction is not a trivial task because of the inherent complexities of subsurface fractures and the generally insufficient geological/geophysical knowledge. We explore using a data assimilation approach, ensemble smoother with multiple data assimilation (ESMDA), to interpreting tracer data for long-term thermal performance prediction in EGS reservoirs. There are three major components in the proposed approach: 1) We use principal component analysis (PCA) to reduce the dimensionality of fracture models. 2) We use ESMDA to assimilate various tracer data (conservative and sorptive tracer) jointly and obtain a posterior ensemble of fracture models. 3) The posterior fracture models are used to perform thermal simulation and predict long-term thermal performance. We developed a field-scale EGS model to verify the capability of the proposed approach in fracture characterization and long-term thermal performance prediction. We also applied the approach to a meso-scale field experiment to further demonstrate its potential application in subsurface reservoir characterization. The results indicate that the long-term thermal breakthrough behavior can be appropriately predicted by assimilating conservative and sorptive tracer data simultaneously.

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MS15 / 203

## Prediction of Flow and Reactive Transport using Physics-Informed Neural Networks

**Authors:** Hongkyu Yoon<sup>1</sup> ; Vincent Liu<sup>1</sup> ; Jonghyun Lee<sup>2</sup>

<sup>1</sup> *Sandia National Laboratories*

<sup>2</sup> *University of Hawaii at Manoa*

**Corresponding Authors:** jonghyun.harry.lee@hawaii.edu, hyoon@sandia.gov, vinliu@sandia.gov

Flow and reactive transport in fractured and porous media are fundamental to understanding coupled multiphysics processes critical to various geoscience and environmental applications such as geologic carbon storage, subsurface energy recovery, and environmental biogeochemical processes. Although fluid dynamics simulations provide fundamental solutions to flow and reactive transport processes, these computational simulations are often computationally intensive and would not be scalable to high dimensional applications. Deep learning can offer computationally efficient solutions to such problems while reliable neural network models require a large number of training samples. Physics-informed neural network approaches can provide machine learning solutions to physical systems respecting the laws of physics given by general nonlinear differential equations with a small number of training data, but training such networks require domain-specific expertise for better convergence. In this work, we apply hybrid physics informed neural networks and data augmentation to predict fluid flow in a constrained geometry. We test our models to evaluate various flow and reactive transport problems in 2D domains using the advection-diffusion(or dispersion)-reaction and Navier Stokes/Darcy equations. Additionally, we test flow and transport problems in the presence of an obstructing cylinder to analyze fluid velocity and concentration distribution from advection-diffusion-reaction. Comparison of results between the physics-informed deep learning approaches and computational simulations will be presented to highlight the accuracy of physics-informed neural networks and advance computational efficiency. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS25 / 141

**Process-dependent solute transport in porous media****Authors:** Hamidreza Erfani Gahrooei<sup>1</sup>; Nikolaos Karadimitriou<sup>2</sup>; Alon Nissan<sup>None</sup>; Monika Walczak<sup>None</sup>; Brian Berkowitz<sup>3</sup>; Vahid.J Niasar<sup>None</sup><sup>1</sup> *University of Manchester*<sup>2</sup> *Institute of Mechanics (CE), Stuttgart University*<sup>3</sup> *Weizmann Institute of Science***Corresponding Authors:** vahid.niasar@manchester.ac.uk, nkaradimitriou@gmail.com, alon.nissan@weizmann.ac.il, hamidreza.erfanigahrooei@postgrad.manchester.ac.uk, monika.walczak@manchester.ac.uk, brian.berkowitz@weizmann.ac.il

Solute transport under single-phase flow conditions in porous micromodels was studied using high-resolution optical imaging. Experiments examined loading (injection of ink-water solution into a clear water-filled micromodel) and unloading (injection of clear water into an ink-water filled micromodel). Statistically homogeneous and fine-coarse porous micromodels patterns were used.

It is shown that the transport time scale during unloading is larger than that under loading, even in a micromodel with a homogeneous structure, so that larger values of the dispersion coefficient were obtained for transport during unloading.

The difference between the dispersion values for unloading and loading cases decreased with an increase in the flow rate. This implies that diffusion is the key factor controlling the degree of difference between loading and unloading transport time scales, in the cases considered here. Moreover, the patterned heterogeneity micromodel, containing distinct sections of fine and coarse porous media, increased the difference between the transport time scales during loading and unloading processes. These results raise the question of whether this discrepancy in transport time scales for the same hydrodynamic conditions is observable at larger length and time scales.

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MS13 / 635

**Progress towards SAXS-based PEFC catalyst layer saturation determination****Author:** Kinanti Hantiyana Aliyah<sup>1</sup>**Co-authors:** Lorenz Gubler<sup>2</sup>; Jens Eller<sup>1</sup><sup>1</sup> *Paul Scherrer Institut*<sup>2</sup> *Electrochemistry Laboratory, Paul Scherrer Institut*



**Corresponding Authors:** jens.eller@psi.ch, aliyah.kinanti@psi.ch, lorenz.gubler@psi.ch

Water management is of high importance to overcome mass transport limitations in polymer electrolyte fuel cells (PEFC) at high current densities. Although the knowledge about water management in the catalyst layer is continuously increasing, it has not been fully understood so far. Within the past decade, numerous methods for *ex-situ* and *operando* imaging of water evolving in the porous structures of the PEFC have been explored, primarily X-ray and neutron imaging methods [1,2]. However, due to the lack of time and/or spatial information of these studies, the catalyst layer saturation mechanism remains unclear.

Here, we propose small angle X-ray scattering (SAXS) as a diagnostic tool for investigating catalyst saturation processes. We confirm that intensity changes in SAXS profiles can be attributed to different pore filling mechanisms with the help of virtual SAXS experiments. A series of experimental studies of *ex-situ* and *in-situ* wetting of catalyst layer was conducted. Stochastic morphological model was used to interpret the data. Derivation of the liquid content inside the catalyst layer was also performed. We believe that the mechanistic knowledge of catalyst layer saturation obtained from this diagnostic tool is essential to move forward materials development for higher performing PEFCs.

#### Time Block Preference:

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1 A. Bazylak, Int. J. Hydrog. Energy. 2009, 34, 3845-3857

[2] P. Boillat et al, Curr. Opin. Electrochem. 2017, 5, 1, 3-10 **Acceptance of Terms and Conditions:**

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MS15 / 21

## Promises, Challenges and Prospects of Deep Learning for Providing Insight into Multi-phase Flow Through Porous Media

**Author:** Seyed Reza Asadolahpour<sup>1</sup>

**Co-authors:** Zeyun Jiang<sup>1</sup> ; Helen Lewis<sup>1</sup> ; Jim Buckman<sup>1</sup>

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The advent of deep learning marked a milestone in the real-life applicability of machine learning tools, as now very complex problems can be solved with unprecedented accuracy. Deep neural networks generally require little explicit prior knowledge and are distinctively efficient in extracting complicated patterns. These capabilities turn them into feasible candidates for replacing and/or assisting conventional time-consuming and computationally-expensive methods involved in pore-scale modelling, such as reconstruction, segmentation and single-/multi-phase simulations.

This work aims to show how the power of deep learning can be harnessed to both estimate porous-media properties and develop new insights. Our main objectives are: (1) provide a general overview of how deep neural networks have already been used in terms of single/multi-phase flow characterization; (2) demonstrate the potentials of deep learning in digital rock physics through case studies; (3) discuss deep-learning-based approaches to explore the physics of the porous media.

First, the relevant body of research is considered so that advancements, gaps and potentials can be identified. Then, an implementation map is laid out, encompassing the simplest to most comprehensive applications. Inputs can range from grey-level images to customized feature maps, while targets can span from static properties to complex, dynamic multi-phase properties (e.g., resistivity index and fluid distribution). Secondly, case studies are presented where porosity, permeability and relative permeability are predicted from micro-CT (e.g., synchrotron beamline) images and rock-fluid

characteristics. A great challenge is to achieve the simulations at representative sample image sizes, which makes hyperparameter sweeping extremely taxing for the researcher and demanding on the hardware.

Thirdly, future research is discussed. It is proposed that to develop reliable multi-phase predictors, large databases must be synthesized by collecting, resampling, augmenting, and grouping images and the corresponding properties. Consequently, deep neural networks can be trained for various rock types (e.g., carbonate) and processes (e.g., two-phase unsteady-state drainage). Singular or ensembles of networks may either be used to make predictions or to serve as the base to be customized for other applications, i.e., transfer learning. Final models can be put to ultimate real-life testing by comparing against experimental data, e.g., phase distributions from synchrotron imaging.

Rather than trying to create mere black-box estimators, one must strive to understand how the networks extract information, by looking at layer architectures, weights and other elements. The goal should be to gain insights into various flow functions (e.g., uncover the link between macroscopic properties and pore morphology and/or wettability) and the physics of certain flow behaviours (e.g., snap-off). This has already been done in such fields as object recognition, for instance, to figure out the level of feature abstraction at different layers. Furthermore, since trained models are very fast to run, they make perfect assets for such tasks as sensitivity/uncertainty analysis and back-calculation of input features, for instance, to see what wettability distribution can result in a specific flow parameter.

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MS6-A / 744

## Quantification of non-linear multiphase flow in porous media for both water-wet and mixed-wet conditions

**Authors:** Yihuai Zhang<sup>None</sup>; Branko Bijeljic<sup>1</sup>; Ying Gao<sup>2</sup>; Qingyang Lin<sup>2</sup>; Martin Blunt<sup>2</sup>

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The flow of multiple fluids in porous materials occurs in a wide variety of important natural and engineered settings relevant for the understanding of geological CO<sub>2</sub> storage, geothermal energy extraction, magma flow, oil and gas recovery, contaminant transport, flow in fuel cells, microfluidics in drug delivery, and the effectiveness of respirators and surgical masks. However, the transition from traditional Darcy flow to non-linear flow is always a ‘mystery’. Here, we measure the pressure differences during two-phase flow across sandstone sample (both water-wet and mixed-wet conditions) for a range of injection rates and fractional flows, during an imbibition experiment. We quantify the onset of a transition from a linear relationship between flow rate and pressure gradient to a non-linear power-law dependence. We show that the transition from linear (Darcy) to non-linear flow and the exponent in the power-law is a function of fractional flow. We use energy balance to propose a new Y number equation, and then the first time accurately predicts the onset of intermittency for a range of fractional flows, fluid viscosities and different rock types.

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Poster + / 540

**Quantification of uncertainty associated with the estimation of hydraulic parameters for saturated porous media****Author:** Sahil Sharma<sup>1</sup>**Co-authors:** Chandni Thakur<sup>2</sup>; Deepak Swami<sup>1</sup>; K S Kasiviswanathan<sup>2</sup><sup>1</sup> *Indian Institute of Technology Mandi*<sup>2</sup> *Indian Institute of Technology Roorkee***Corresponding Authors:** chandnithakur2@gamil.com, deepak@iitmandi.ac.in, kasifwt@iitr.ac.in, sharmasahilbuce@gmail.com

Estimation of subsurface hydraulic parameters is always complicated often due to lack of the available information. For the reliable estimation of the hydraulic parameters i.e. hydraulic conductivity (Ks) and porosity ( $\Theta$ s), experiments are conducted at lab scale but for field scale it's expensive, time consuming and not feasible. The alternative approach is to use empirical relation based on physical properties of the aquifer material. Since these empirical relation are well established and are used extensively for the estimation of in-situ hydraulic parameters. This study is conducted to highlight the uncertainties associated with various empirical relations for the estimation of hydraulic parameters of heterogeneous porous medium. During the estimation of input parameters for these empirical relations, spatial variability in soil characteristics along with interpolation error, unsteadiness of flow and the instrument calibration errors impose varying degrees of uncertainty. Classical uncertainty methods such as zero order, first order and second order uncertainty were applied to empirical equations that were often used for estimating hydraulic conductivity in groundwater flow modeling. The combination of uncertainty quantification method with different empirical equations lead to several cases which were compared for the variance and mean estimates to identify the model of less uncertainty along with reliable mean estimate of hydraulic conductivity. The values of the hydraulic parameters obtained from the empirical equations are then compared with the experiments conducted on three mini aquifer systems i.e. glass beads, sand and soil. Further the applicability of various empirical equations were delineated with the experimental results for a particular mini aquifer system. It is concluded from results that the uncertainty estimated from second order was more as compared to the first order uncertainty method, however mean value of Ks estimate was in close range. Further, we found that applying second order uncertainty is computationally complex which leads to the application of first order uncertainty analysis. Nevertheless, comprehensive evaluation of various uncertainty method is crucial in groundwater flow modeling especially for the parameters of high variability such as considered here.

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Poster + / 746

**Quantifying Evolution of Mineral Reactive Surface Area and Pore Connectivity for Improved Prediction of Mineral Reaction Rates in Porous Media****Authors:** Md Fahim Salek<sup>1</sup>; Fanqi Qin<sup>None</sup>; Lauren Beckingham<sup>1</sup>

<sup>1</sup> Auburn University

**Corresponding Authors:** leb0071@auburn.edu, fzq0004@auburn.edu, mzs0184@auburn.edu

Understanding mineral reaction rates in porous material is crucial in many environmental systems such as natural weathering process, enhanced oil recovery, radioactive waste disposal etc. Prediction of in-situ mineral reaction rates is challenging, and a significant variation is observed between laboratory data compared to field data due to factors like variation in the physicochemical properties of minerals, spatial heterogeneities, chemical composition of the fluid, etc. Previous studies have suggested that this discrepancy is mostly due to the imprecision in determining the mineral reactive surface areas. Even in many cases, the evolution of surface areas of different mineral phases during the reaction gets ignored. Core flood experiments under acidic condition can provide information about the geochemical reactions, mineral dissolution-precipitation kinetics, and surface area evolution. In this study, a brine solution mixed with HCl is injected into a sandstone core sample from the Torrey Buff formation. 3D X-ray nano-computed tomography (X-ray nano-CT) imaging and Scanning Electron Microscopy (SEM) Backscattered electron (BSE) and Energy-dispersive X-ray spectroscopy (EDS) images are used to determine the mineral volume fractions, connected porosity, and accessible mineral surface areas as reactions progress. A reactive transport simulation is carried out in a multicomponent reactive flow and transport modeling tool, CrunchFlow, to simulate reaction rates and the evolution of mineral volume fractions and accessible surface areas. Finally, simulation results are compared with results achieved from the core flood experiment and X-ray imaging outputs.

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MS5 / 652

## Quantifying sulfate reduction rates of biofilm on shale fracture walls within a microfluidic reactor

**Authors:** Lang Zhou<sup>1</sup> ; Ananda S Bhattacharjee<sup>None</sup> ; Glenn A Fried<sup>None</sup> ; Mayandi Sivaguru<sup>None</sup> ; Kyle Michelson<sup>None</sup> ; Robert A Sanford<sup>None</sup> ; Bruce W Fouke<sup>None</sup> ; Charles J Werth<sup>None</sup>

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**Corresponding Authors:** werth@utexas.edu, kylemi85@gmail.com, fouke@illinois.edu, langzhou@utexas.edu, asbhatta@illinois.edu, rsanford@illinois.edu, sivaguru@illinois.edu, gfried@igb.uiuc.edu

During hydraulic fracturing, preferential flow paths are created to extract hydrocarbons from shale reservoirs, typically with large amounts of produced water. The water is often rich in hydrocarbons and sulfate, providing ideal nutrients for promotion of sulfate reducing bacteria (SRB) growth and biosouring. Bacteria growth may clog fracture pathways and decrease hydrocarbon production, while biosouring represents a pipeline corrosion and human health hazard that can shut down production. In this work, a natural shale sample is shaped to create two inlets that feed into a single 250  $\mu\text{m}$ -wide fracture, all contained within a microfluidic platform. Hydrocarbon fermentation products (i.e., fatty acids) are fed into one inlet, and sulfate into the other; they mix in the fracture and promote biomass growth and sulfate reduction. SRB biofilms on shale fracture walls are quantified using bright-field microscopy and image analyses, and sulfate reduction is quantified using a zinc trap to capture effluent sulfide. A numerical model is developed to interpret the biomass growth results, and to quantify sulfate reduction rates. These rates are compared to those reported in the literature for batch experiments, and recommendations for accurately modeling sulfate reduction in shale fractures are proposed.

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MS3 / 376

## Quantifying the corrosive influence of water and carbon dioxide on crack propagation in silica

**Authors:** Filip Simeski<sup>1</sup> ; Matthias Ihme<sup>1</sup> ; Alireza Ostadhossein<sup>1</sup><sup>1</sup> *Stanford University***Corresponding Authors:** ostadhossein.hanif@gmail.com, mihme@stanford.edu, filip.simeski@stanford.edu

The stimulation of crack growth in quartz and siliceous materials by hydraulic fluids or carbon dioxide (CO<sub>2</sub>) injection remains an open issue when assessing the production of natural gas wells and long-term carbon storage. In this work, we employ reactive molecular dynamics (MD) simulations to study how the fluid environment (specifically, CO<sub>2</sub> or water) affects the mechanical properties of pre-cracked quartz grains. The thermodynamic conditions of interest are those relevant to subsurface reservoirs. Results from this study suggest that water and CO<sub>2</sub> substantially reduce the fracture toughness of quartz, thereby promoting crack growth and enhancing fluid transport in the subsurface. We report on how structural properties – bond length distribution and crack tip shape – evolve upon introduction of a fluid. These properties directly relate to macroscopic quantities of the global stress-strain curves, thus reaffirming the inherent coupling across multiple scales for fluid-solid interactions in the subsurface. Finally, the application of reactive MD simulations allows us to discuss the molecular processes that are causal for the observed chemo-mechanical processes at the continuum scale. The implications of this work may inform design principles for climate change mitigation technologies, including carbon sequestration, enhanced geothermal systems, and energy storage.

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MS3 / 664

## Quick estimation of capillary pressure barrier of fractured caprocks.

**Authors:** Christine Maier<sup>1</sup> ; Rafael March<sup>1</sup> ; Niko Kampman<sup>2</sup> ; Kevin Bisdom<sup>2</sup> ; Florian Doster<sup>1</sup><sup>1</sup> *Heriot-Watt University*<sup>2</sup> *Shell Global Solutions International B.V.***Corresponding Authors:** kevin.bisdom@shell.com, niko.kampman@shell.com, f.doster@hw.ac.uk, rafaelmarch3@gmail.com, c.maier@hw.ac.uk

An ideal CO<sub>2</sub> storage site needs to be able to contain a large volume of CO<sub>2</sub> without any significant leakage through the caprock seal. Aside from legacy wells, (sub-seismic) faults and associated fractured damage zones form a potential containment risk. A well-connected fracture network can increase the permeability and decrease the capillary barrier of the caprock, rendering them to be potential pathways for CO<sub>2</sub> leakage. Therefore, for a successful identification of sequestration sites, quick screening of fault-related leakage risks is needed. In this work we present a workflow to quickly estimate the capillary pressure barrier of a fault related fracture network under different stress conditions using percolation algorithms on two different scales, the single fracture scale, and the fracture network scale.

For the fracture scale we generate several synthetic fracture surfaces with different roughness values and calculate the resulting aperture field. This aperture field informs a capillary entry pressure field via the Young-Laplace equation. The proposed algorithm determines if a percolation of CO<sub>2</sub> from one boundary of the fracture to another occurs for specific fluid pressure values at the inlet. The fluid pressure at percolation is then defining the upscaled capillary entry pressure of the fracture. This procedure is repeated for a range of stress boundary conditions acting on the fracture walls, that is for different average fracture apertures, to obtain the stress sensitive capillary entry pressure relationship for fractures with different roughness properties.

On the fracture network scale, we apply a similar upscaling procedure on various statistical realisations of a fault related fracture network. Different stress values on the fracture network boundaries determine the stresses acting on each individual fracture of the network. Using these stress values and the corresponding upscaled capillary entry pressures from the previous step informs a heterogeneous capillary pressure field of the whole network that then can be used to obtain the uncertainty envelope for the overall fracture network capillary pressure barrier.

Low values of capillary pressure barrier would indicate higher leakage risk associated with that site. High values on the other hand, could identify a potential storage site that needs further investigations to determine its 'quality'. The proposed algorithms are computationally very efficient and thus provide with a powerful tool for rapid screening of potential CO<sub>2</sub> sequestration sites.

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## **RHEOLOGICAL RESPONSE OF FOAM FLOODING MODELS CONSIDERING EXPERIMENTAL UNCERTAINTIES**

**Authors:** Andres Valdez<sup>1</sup> ; Bernardo Rocha<sup>2</sup> ; Grigori Chapiro<sup>3</sup> ; Rodrigo Weber<sup>2</sup>

<sup>1</sup> *PhD candidate in computational modeling*

<sup>2</sup> *Professor*

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**Corresponding Authors:** grigorichapiro@gmail.com, rodrigo.weber@uff.edu.br, arvaldez@ice.uff.br, bernardo-martinsrocha@ice.uff.br

In this work, we study uncertainties originating from foam flood models' responses concerning non-Newtonian behavior. This work presents how uncertainty affects foam rheology and analysis of Newtonian and non-Newtonian foam formulations. To this end, the Markov Chain Monte Carlo (MCMC) technique was used to estimate parameters for the different foam models. In addition, a global sensitivity analysis based on Sobol indices was also performed to determine which input parameter is more relevant to variations in the quantities of interest. The quantities of interest are apparent viscosity, mobility reduction factor, and total relative mobility, among others. Experimental data were obtained from the literature for the Bayesian parameter estimation of the STARS models. In particular, to focus on Newtonian and non-Newtonian behavior, we adopted the STARS model with its dry-out component and shear thinning function. The results indicate how much the choice

of a specific model for foam flow (Newtonian or non-Newtonian) can be affected by uncertainties from estimated parameters.

**Acknowledgements:** The current work was conducted in association with the R&D project ANP n° 20715-9, “Modelagem matemática e computacional de injeção de espuma usada em recuperação avançada de petróleo” (UFJF/Shell Brazil/ANP). Shell Brazil funds it in accordance with ANP’s R&D regulations under the Research, Development, and Innovation Investment Commitment. This project is carried out in partnership with Petrobras.

**Time Block Preference:**

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A. R. Valdez, B. M. Rocha, G. Chapiro, and R. W. dos Santos. Uncertainty quantification and sensitivity analysis for relative permeability models of two-phase flow in porous media. *Journal of Petroleum Science and Engineering*, 2020. doi: 10.1016/j.petrol.2020.107297

F. F. de Paula, T. Quinelato, I. Igreja, and G. Chapiro. A numerical algorithm to solve the two-phase flow in porous media including foam displacement. In *Lecture Notes in Computer Science*, volume 12143, pages 18–31. Springer, 2020. doi: 10.1007/978-3-030-50436-6\_2

A. Valdez, B. Rocha, A. Pérez-Gramatges, J. Façanha, A. de Souza, G. Chapiro, and R. dos Santos. Foam assisted water-gas flow parameters: from core-flood experiment to uncertainty quantification and sensitivity analysis. *Transport in Porous Media*, 2021. doi: 10.1007/s11242-021-01550-0

L. F. Lozano, R. Q. Zavala, and G. Chapiro. Mathematical properties of the foam flow in porous media. *Computational Geosciences*, 25(1):515–527, 2021. doi: 10.1007/s10596-020-10020-3 **Acceptance of Terms and Conditions:**

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MS9 / 14

## Random Emulation of Large-Scale Natural Pore Networks

**Author:** Daniel Meyer<sup>1</sup>

<sup>1</sup> *Institute of Fluid Dynamics, ETH Zurich*

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Over the past years, tomographic scanning techniques like micro-CT have enabled the acquisition of high-fidelity void-space geometries of natural porous media [e.g., Raeini, Bijeljic, and Blunt, *Physical Review E*, 96, 1 (2017)]. There are, however, experimental/computational limitations in the sample size, respectively level of detail or voxel count, that can be acquired [Section 2.3 in Cnudde and Boone, *Earth-Science Reviews*, 123 (2013)]. Moreover, limitations both in computing time and memory prohibit direct numerical simulation (DNS) of flow and transport in large resp. detailed sample geometries. Pore networks derived from scans alleviate this second limitation or computational burden, but introduce model assumptions and still necessitate a methodology to extrapolate to larger samples. Such a methodology is needed, especially for relatively inhomogeneous rocks like carbonates, as the scales of representative elementary volumes (REV) for flow and transport theories are often larger than the sample sizes that are currently scanned/post-processed [Meyer and Bijeljic, *Physical Review E*, 94, 1 (2016)].

In this work, we address this need by presenting a new pore network generation algorithm. While emulating from an existing base network new networks of equal or larger sizes, the new algorithm scales approximately linearly with the pore count and maintains (1) pore coordination-number statistics, (2) geometrical pore/throat properties, as well as (3) the potentially inhomogeneous spatial clustering of pores. While existing methods address the first two properties [Idowu, *Pore-Scale Modeling*:

Stochastic Network Generator and Modeling of Rate Effects in Waterflooding, Imperial College London (2009)], the third point is crucial to match flow/transport properties such as the permeability in inhomogeneous media.

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MS7 / 369

## Random Walks and Simplified Marching Cube for image-based simulations of heat or mass transfer in evolving porous media and applications to Ceramic-Matrix Composites

**Author:** Gerard Vignoles<sup>1</sup>

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Simulation problems linked to the fabrication and degradation of Ceramic-Matrix Composites involves a precise knowledge of effective heat and mass transfer properties of porous media at the fiber scale and the fabric scale. When dealing with complex reinforcement architecture, predictive tools have to be able to handle large 3D images, including the capability to modify them through infiltration or ablation phenomena. This presentation will describe a class of methods developed to fulfil these requirements. Monte-Carlo/Random Walks have the interesting property of simulating diffusive, ballistic or mixed-mode transfer phenomena in a straightforward way. Moreover, they require a very small amount of extra memory in addition to image storage, thus enabling simulations in very large images. Coupled to an efficient interface discretization scheme, the Simplified Marching Cube, they are very efficient.

Example of applications to simulations of Chemical Vapor Infiltration, featuring rarefied gas transfer, chemical deposition and porous medium densification, and to simulations of conducto-radiative heat transfer in fibrous media will be given, in order to illustrate the versatility and performance of this class of methods.

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## Rapid spreading of complex fluids in porous substrates

**Author:** Prashant Agrawal<sup>1</sup>

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With the advent of paper microfluidics and the concept of Point-of-care healthcare diagnostics, study of imbibition of complex fluids in porous media has become significantly important. In these applications, a rapid and even spread of complex fluids on absorbent paper is essential to ensure a uniform component spread for accurate chemical and bio-sensing. Especially in the case of blood analysis techniques like Dried Blood Spot (DBS) analysis, an even and rapid spread of blood is crucial to avoid coagulation and even distribution of analytes for consistent sample spotting. While cellulose-based filter papers, commonly used in these applications, are good for absorption, the nanoporous matrix provides a significant hindrance to the flow of a liquid. Thereby, it inhibits the spread of a liquid. The porous network can also clog if the fluid contains large particulate matter.

In this work we present a filter paper based device where we overcome the resistance to fluid flow which allows a rapid and even spread of complex liquids. In our design, we sandwich a filter paper between a nanofibrous matrix supported on a polyethylene terephthalate (PET) sheet. With this sandwich design, we decrease the net resistance to the flow while maintaining the high suction pressure provided by the filter paper. As a result, a large quantity of liquid can be imbibed into the device quickly and evenly. We demonstrate the working of this device for linear imbibition using three types of liquids: dyed water, milk solutions and whole blood. We support these experimental observations using a 1D Darcy's law for flow in porous media. We also employ a simple equivalent resistance model to demonstrate how the sandwich design reduces resistance to flow compared to just the filter paper.

The concepts and designs presented in this work can be expanded to radial imbibition for use in microfluidic devices. As the design relies on additive manufacturing, without any modifications to the source paper, the concepts can also be used for improving the reliability of Dried Blood Spotting techniques.

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MS8 / 576

## Rayleigh-Taylor Instability in 2D and 3D Dispersive Porous Medium

**Authors:** Jayabrata Dhar<sup>1</sup> ; Patrice Meunier<sup>2</sup> ; François Nadal<sup>3</sup> ; Yves Méheust<sup>1</sup>

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CO<sub>2</sub> injected in deep saline aquifers for subsurface carbon sequestration is supercritical (sCO<sub>2</sub>), and thus less dense than the resident brine. The plume of sCO<sub>2</sub> to the top of the formation and widens under the cap rock, where it is placed above the brine. Due to its partial solubility in the brine, sCO<sub>2</sub> dissolves into it, leading to the formation, at its interface with the brine, of an aqueous mixture which is denser than the brine. A gravitational instability then develops, and the convection that ensues allows dissolved CO<sub>2</sub> to be transported deeper into the formation, where it remains trapped by gravity. The convection also puts the sCO<sub>2</sub> with CO<sub>2</sub>-devoid brine, which nurtures the dissolution process. This convective dissolution in essence results from the coupling between dissolution

of  $s\text{CO}_2$  into the aqueous phase, buoyancy-triggered flow of the latter phase, and transport of the dissolved  $\text{CO}_2$  within it. When modeled at the continuum (i.e., Darcy) scale, the solute transport equation must take into account dispersion. Continuum scale numerical simulation of convective dissolution has attracted much attention; many of these previous studies have considered simple diffusive transport (i.e., a constant diffusion/dispersion coefficient in the transport equation), and few of them have tackled three-dimensional (3D) geometries. We present a numerical investigation, based on the open source numerical toolbox OpenFOAM associated to a custom-written solver relying on the stream function, of convective dissolution in two-dimensional (2D) and 3D geometries, taking into account dispersive transport through a classic anisotropic dispersion tensor proportional to the local Darcy velocity and featuring two main parameters: (i) the dispersion's strength (as compared to molecular diffusion), and (ii) the ratio of the longitudinal dispersivity to the transverse dispersivity. A systematic study was performed as a function of these two parameters and of the Rayleigh number, which quantifies the relative importance of convection-controlled advective transport and dispersive transport. The convective dissolution process is characterized in terms of the onset times of the linear instability and of nonlinear convection, the number density of convective fingers, and the associated flux of dissolved  $\text{CO}_2$ . The onset time of nonlinear convection is found to strongly depend on the Rayleigh number, but not of the intensity of dispersion. However the two parameters characterizing dispersion have a strong influence on the global time scale of  $\text{CO}_2$  dissolution. We also discuss the differences in convective finger structures between the 2D and 3D geometries, and their consequences on the convective dissolution process.

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MS6-A / 318

## Re-evaluation of the evolution and hysteresis of relative permeability in gas-brine systems: time to shift the paradigm?

**Authors:** Michael Clennell<sup>1</sup>; Samuel Jackson<sup>1</sup>; Mojtaba Seyyedi<sup>1</sup>

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Predicting injectivity, well productivity, trapping effectiveness and storage efficiency in subsurface reservoirs or saline aquifers requires a good understanding of how relative permeability changes with fluid saturation. While exact values of gas permeability at any given saturation are unknown, practitioners often assume that the general form of relative permeability curves are predictable and unlikely to deviate from the norm.

The “norm” for gas-brine relative permeability curves we call the Brooks-Corey-van Genuchten Paradigm:

1. Drainage gas-brine relative permeability curves for both the non-wetting gas phase and for water have a concave-upwards shape and can be fit with a power law function.
2. Imbibition relative permeability curves for the gas phase have the same concave upwards shape (possibly with a different exponent).
3. Imbibition curves for gas relative permeability always lie below the primary drainage curve, terminating in a value of residual saturation that depends on the maximum saturation of gas reached during drainage.

We examined the evidence for the universality of the B-C-vGn paradigm, based on understanding gained from recent literature, by revisiting alternative concepts and by reviewing experimental and modelling studies. We found good evidence for drainage relative permeability curves that commence with a concave-upwards shape but that flatten off towards irreducible water saturation to have an overall ‘S’ shaped profile. Network models suggest this shape is prevalent in strongly water wet systems. We have also measured directly brine-gas imbibition relative permeability curves in sandstones and found a convex-upwards shape that loops back over the primary drainage curve to the

end point marking residual gas saturation. We found several published experimental curves with this pattern in a range of soils and rocks, and validation from from percolation theory and network modelling that this form is to be expected in water wet systems including many methane, hydrogen and CO<sub>2</sub> storage scenarios.

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MS22 / 218

## Reaction-induced changes to structure and transmissivity of foamed wellbore cements

**Authors:** Johnathan Moore<sup>1</sup> ; Magdalena Gill<sup>1</sup>

**Co-authors:** Dustin Crandall<sup>2</sup> ; Richard Spaulding<sup>2</sup> ; Barbara Kutchko<sup>2</sup>

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Foamed cement is used in deep well construction for its strength, versatility, and ease of density adjustment by changing the gas fraction during slurry injection. When well cement is fractured it may encounter formation and injected fluids. Understanding potential reaction-induced changes in wellbore cement is crucial to managing well integrity in these situations.

To examine the alteration of a fractured foamed cement in a geologic carbon storage system, six Portland class H foamed cement samples were created with different gas fractions, fractured, and exposed to flowing CO<sub>2</sub>-acidified water (carbonic acid) over a period of several days. The experiments were conducted at room temperature, under a confining pressure of 8.27 MPa, pore pressure of 5.52 MPa, and were periodically imaged with a Computed Tomography (CT) scanner. The differential pressure across the sample was measured during the experiment to evaluate changes in fracture conductivity. Image analysis of the progressive changes in the matrix shows that foamed cements are a heterogenous material with varying degrees of susceptibility to reactive liquids. The transformation of cement matrix suggests both matrix dissolution and mineralogic alteration play a part as the reaction front migrates through the sample, with principal reacted zones residing in the immediate vicinity of the fracture. We present a discussion of the morphological changes observed in CT data in the cement matrix, coupled with an analysis of simulated fluid flow paths through the altered fracture geometry and transmissivities as the cement matrix reacts with carbonic acid.

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MS1 / 494

## Reactive CO<sub>2</sub> Density-Driven Flow in Aquifers

**Authors:** Hamidreza Erfani Gahrooei<sup>1</sup> ; Masoud Babaei<sup>1</sup> ; Vahid.J Niasar<sup>None</sup>

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The dissolution of carbon-dioxide (CO<sub>2</sub>) in deep saline aquifers is an important trapping mechanism in carbon storage. This process is triggered by unstable high-density CO<sub>2</sub> front, which later promotes density-driven mixing, hydrodynamic dispersion of CO<sub>2</sub> and favors the long-term sequestration. In many former studies, the effects of hydrodynamic dispersion and multispecies geochemical reactions have been ignored.

This work elaborates the impacts of these simplifications on the dynamics of convective mixing by numerical simulations. Geochemical effects were studied by the implementation of rock-fluid and fluid-fluid interactions for typical sandstone and carbonate aquifers. Results show that accounting for the hydrodynamic dispersion decreases the convection onset time and increases the CO<sub>2</sub> dissolution flux, which is more significant in larger dispersivities and Rayleigh numbers. Results indicate that carbonate geochemical reactions intensify the long-term overall efficiency of the process, while decrease the total amount of sequestered carbon in the diffusion-dominated period. Conversely the sandstone geochemical interactions were shown to have a different impact on the process compared to carbonate interactions. Results also reinforce the importance of realistic geochemical representation and the importance of spatial and temporal dependence of the reactions pathway, subsequent to the finger development for more detailed simulation of the CO<sub>2</sub> storage process.

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MS9 / 82

## **Reactive Imbibition of Acidic Fluids in Unconventional Shales: A New Experimental Approach to Pore-Scale Reactive Transport Modeling**

**Author:** Vincent Noel<sup>1</sup>

**Co-authors:** Jennifer Druhan<sup>2</sup> ; Florent Brondolo<sup>1</sup> ; Wenjia Fan<sup>3</sup> ; Anthony Kovscek<sup>3</sup> ; John Bargar<sup>1</sup> ; Gordon Brown<sup>3</sup>

<sup>1</sup> *SLAC National Accelerator Laboratory*

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Imbibition – the process of a wetting fluid displacing a nonwetting fluid in porous media – profoundly affects geochemical reaction networks in stimulated geological formations. Current quantitative models of fluid transport in such formations widely assume that imbibition of fluids into porous media occurs on a faster time scale than geochemical reaction front evolution. This assumption provides a considerable simplification of an otherwise highly complex reactive transport problem. Yet a body of literature suggests that the rates of fluid transport, porosity generation, and geochemical reactions may be coincident and closely coupled during the imbibition process [1-3], with implications for geological stimulation strategies.

Here, we report direct temporal and spatial observations of contemporaneous porosity modification and fluid imbibition within shale cores in contact with acidic aqueous fluids commonly used in fracture stimulation processes. To obtain these data, we tracked acidic fluid transport in shales by monitoring the rate and spatial extent of bromide tracer transport using synchrotron X-ray fluorescence mapping combined with compositional analysis of the bulk acidic hydraulic fracturing fluids (HFFs). Our approach yields a direct record of time-resolved selective ion transport resulting from the penetration of HFFs and attendant mineral transformations. Our experiments highlight that the penetration of acidic HFFs and calcite dissolution occur at similar rates in oil/gas shales, and indicate that reaction fronts evolve rapidly during imbibition of HFFs. We also show that the variability in mineralogy and chemical reactivity of shales can directly affect the rate and spatial extent of imbibition. For example, although the reaction of the acid spear head with carbonates in shales enhances calcite dissolution and increases porosity, the spatial extent of calcite dissolution in the shale matrix is limited due to a rapid neutralization of pH. In addition, rapid secondary mineral precipitation, such as precipitation of Ba-bearing minerals, reduces porosity and helps explain the significant reduction in the spatial extent of the reaction front and the lower rate of fluid imbibition. Although models of fluid-shale interactions frequently omit a direct feedback between imbibition and reactive chemical/mineralogical alteration of pore structure, our study demonstrates that neglecting geochemical reactivity and pore space modification during imbibition will create major uncertainties in model simulations and potentially impacted the performance and associated risks of subsurface stimulation technologies.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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## Reactive Transport Modeling of Nanocapsules for Controlled Release of Cross-linking Agents for Conformance Control

**Authors:** Hamed Mohammadnejad<sup>1</sup> ; Kurt D. Pennell<sup>2</sup> ; Linda M. Abriola<sup>2</sup>

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Nanotechnologies have recently been proposed for use in conformance control applications to modulate the release of cross-linking agents, facilitating deeper placement of polymer-gel systems. In any potential nanotechnology application for improved conformance, large-scale nanocapsule mobility (100s of meters or more) and precise control of crosslinking agent release rate or time (up to few weeks) are essential. These requirements make full-scale experimentation for application design infeasible. Since pilot studies will also be very expensive, test design, performance evaluation,

and optimization will need to be completed using laboratory-validated and calibrated mathematical simulators.

The goal of this work is to develop and evaluate a mathematical model for the simulation of nanocapsule conformance control applications in large-scale heterogeneous formations. The model incorporates nanocapsule and co-injected polymer transport and attachment, controlled release of cross-linking agents from the nanocapsule shell, and subsequent gelation processes. Illustrative simulations are presented for hypothetical inter-well nanocapsule injection tests within heterogeneous subdomains of a statistically simulated reservoir (Stanford VI) [2, 3]. These subdomains exhibit a wide range of petrophysical properties, as well as a dense sampling (25m x 25m x 1m grid blocks) of the entire 3.75km x 5km x 200m domain. Constituent attachment/sorption and gel rheology modules were developed based on calibration to laboratory column and batch experiments performed in similar systems or found in the literature. Pre- and post-treatment tracer and nanocapsule injection scenarios were simulated in a series of inter-well injection-extraction tests to identify conditions that would maximize technology performance, i.e. reduce water cut and maximize sweep efficiency of the post gelation tracer. A model sensitivity analysis is used to highlight the impact of nanocapsule attachment, crosslinker release mechanisms, and gel strength on conformance control performance. The simulation results show that the conformance efficiency strongly depends on high nanocapsule mobility and that additional processes, such as co-polymer injection [4], maybe needed to further improve system performance.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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**MS18 / 685**

## **Reconstructing contaminant release function in a sandbox experiment**

**Authors:** J. Jaime Gómez-Hernández<sup>1</sup> ; Zi Chen<sup>2</sup>

<sup>1</sup> *Universitat Politècnica de València*

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The ensemble smoother with multiple data assimilation is used to reconstruct the release of a contaminant into a sandbox using concentration observations downgradient from the release point. The algorithm is tested first with some synthetic experiments mimicking the sandbox and then applied

to two experiments with different release functions. The frequency of the sampling, the density of the observations, and the magnitude of the observation error play important roles in the proper reconstruction of the source function.

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## Reconstruction of 3D shale digital rock based on generative adversarial network

**Authors:** Yongfei Yang<sup>1</sup> ; Fugui Liu<sup>None</sup> ; Jun Yao<sup>1</sup> ; Huajun Song<sup>None</sup> ; Min Wang<sup>None</sup>

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The pore structure of shale oil reservoir is complex, and the shale cores are hard to acquire. Accurately characterizing the pore structure of shale reservoir is the key to study the fluid seepage law in shale reservoir. Based on the three-dimensional focused ion beam scanning (3D-FIB-SEM) images of real shale cores, the structure of the original generative adversarial network model is redesigned. At the same time, to ensure that the reconstruction results can fully reflect the pore structure information of the shale core, the size of the training sample is increased, and the model is trained to generate three-dimensional shale digital rock. The porosity of the reconstructed digital rock and the original core are compared, and the pore network model is extracted from the reconstructed digital rock, then the pore structure properties are analyzed. The porosity, pore and throat sizes, connectivity, and coordination relationship of the reconstructed digital rock are highly in agreement with the original cores, which verifies that the generative model can generate high-quality three-dimensional shale digital rock. Finally, several digital rocks are generated, and the mean value and variation range of various pore structure parameters are calculated. It is proved that the generated digital rocks have stable pore space characteristics, and the trained generative model has good stability.

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MS22 / 153

## Redox Flow Battery operation may be limited by “Hot Spots” observed in pore scale simulation of flow in carbon fibre felt electrodes

**Authors:** Edo Boek<sup>1</sup> ; Rhodri Jervis<sup>2</sup> ; Farrel Gray<sup>3</sup>

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<sup>2</sup> *UCL*

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The Vanadium Redox Flow Battery (VRFB) is one of the most promising Electro-Chemical Device (ECD) technologies for large scale local storage of renewable energy, such as wind and solar. Commercial exploitation of this technology has emerged, but a lack of fundamental understanding regarding VRFB operation is limiting the development of this new technology. In particular, the energy density must be improved. For this reason, we investigate here the performance of carbon fibre electrode materials using a combination of computational modelling and experimental characterisation. In particular, the surface area of the porous electrode is critical to the device performance. To optimize electrochemical reactions in the electrode, the reactive surface area has to be as large as possible. In terms of micro-structure, this means that the felt fibres must be distributed homogeneously. In current VRFB technology, however, the felts are woven bundles of fibres yielding a large local variation in voids and bundles. Recently, synchrotron micro-CT scanning was used to image the 3D pore structure of a graphite felt in-operando. However, the resulting alteration of the flow field could not be quantified, as it is difficult to measure in-situ due to limited spatio-temporal resolution. Also, it is difficult to obtain the altered flow field from average tortuosity and porosity calculations, as the relation between permeability and tortuosity / porosity is only known empirically. Here we calculate the relation between flow and altered micro-structural properties using direct flow calculations in pore space images of a representative volume of a carbon fibre material obtained from micro-CT imaging. We consider a 3D fibre felt geometry, obtained from micro-CT experiments, and the corresponding flow field, as a test for large volume calculations. The flow field was calculated using our home-grown Lattice-Boltzmann (LB) code (see [4]) on a big data set of 15 billion voxels using HPC facilities. We observe that the electrolyte is concentrated in local areas (“hot spots”), thus limiting electrochemical reactions. The heterogeneity of the commercial soft carbon fibre material may reduce the efficiency of the electrode, due to high voltage spots and damage in the electrode. In addition, under certain electro-chemical conditions, H<sub>2</sub> and O<sub>2</sub> gas bubbles may develop in the pore space of the heterogeneous electrode, which has a detrimental effect on VRFB performance [1]. Therefore we extend our multi-phase LB code to investigate the development of gas bubbles in the electrode (Fig.1b), initially by seeding random gas bubbles, based on our previous work on multi-phase flow in natural porous materials [2,3]. To mitigate problems associated with the heterogeneous nature of carbon fibre graphite felts, we propose a rational design approach to develop new carbon materials with superior properties.

#### **Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

[1] Jervis, R., Brown, L.D., Neville, T.P., Millichamp, J., Finegan, D.P., Heenan, T.M., Brett, D.J. and Shearing, P.R., (2016) *Journal of Physics D: Applied Physics*, 49(43), p.434002

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[3] Zacharoudiou, I., Chapman, E., Boek, E.S. & Crawshaw, J. (2017) “Pore-filling events in single junction micro-models with corresponding lattice Boltzmann simulations”, *Journal of Fluid Mechanics*, 824, 550-573. doi:10.1017/jfm.2017.363

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MS7 / 125

## **Reduced-dimensional models for flow in fractured porous media**

**Authors:** Florian List<sup>1</sup> ; Florin Adrian Radu<sup>2</sup> ; Iuliu Sorin Pop<sup>3</sup> ; Koondanibha Mitra<sup>4</sup> ; Kundan Kumar<sup>5</sup> ; Stephan B. Lunowa<sup>6</sup>



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In a fractured porous medium, the fractures are often characterised by their anisotropic shape. For example, in a two-dimensional situation, the fractures are long and thin formations, in which the medium properties may differ considerably when compared to the corresponding ones in the adjacent blocks. For the numerical simulation of flow in porous media, a commonly adopted strategy is to consider the fractures as reduced-dimensional objects, in this specific case as one-dimensional manifolds. In doing so, two aspects need to be clarified: which mathematical model should be considered inside the reduced-dimensional fracture, and how is this coupled to the mathematical model adopted in the blocks.

In this talk, we discuss these aspects, based on the properties of the porous medium and on the underlying flow models. More precisely, we use the aspect ratio of the fracture as an anisotropic, two-dimensional object, identified below as  $\varepsilon$  (a small, positive parameter). Depending on how the ratio of the porosities in the fracture and in the blocks, respectively of the permeabilities in the two media, scale with  $\varepsilon$ , we identify various situations leading to different reduced-dimensional models in the fracture. We conclude by discussing numerical aspects related to this procedure.

#### **Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

Florian List, Kundan Kumar, Iuliu Sorin Pop, Florin Adrian Radu, Rigorous Upscaling of Unsaturated Flow in Fractured Porous Media, *SIAM J. Math. Anal.* 52 (2020), 239–276.

Kundan Kumar, Florian List, Iuliu Sorin Pop, Florin Adrian Radu, Formal upscaling and numerical validation of unsaturated flow models in fractured porous media, *J. Comput. Phys.* 407 (2020), 109138

S.B. Lunowa, I.S. Pop, B. Koren, Linearized domain decomposition methods for two-phase porous media flow models involving dynamic capillarity and hysteresis, *Comput. Methods Appl. Mech. Eng.* 372 (2020), 113364

D. Seus, K. Mitra, I.S. Pop, F.A. Radu, C. Rohde, A linear domain decomposition method for partially saturated flow in porous media, *Comput. Methods Appl. Mech. Eng.* 333 (2018), 331-355. **Acceptance**

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MS6-A / 473

## **Regimes of fluid-driven grain transport in a confined channel**

**Authors:** Miles Morgan<sup>1</sup> ; David James<sup>1</sup> ; Bjornar Sandnes<sup>1</sup>

<sup>1</sup> *Swansea University*

**Corresponding Authors:** m.l.morgan@swansea.ac.uk, b.sandnes@swansea.ac.uk, d.w.james@swansea.ac.uk

The flow of grains through confined and constricted geometries occurs in an array of industrial and natural settings. As such, various flow configurations have been extensively studied in dry and wet systems, for instance silo, Couette, avalanche and Poiseuille. Here we present experiments in

which fluid-driven, non-buoyant grains, filling a horizontal channel confined from both the sides and above, are found to exhibit a variety of behaviours depending on the imposed flow rate and the size of the channel. For example, at low imposed flow rates the fluid stress from the injected fluid was not sufficient to mobilise the frictional grains and flow akin to Darcy's Law was observed. Above a critical threshold however, grains began to flow at the top of the channel with Gaussian velocity profiles that were self-similar with respect to flow rate, in contrast to the exponential decay seen in bedload transport. These Gaussians became faster with increased flow rate, also penetrating further into the packing. Beyond this regime at high flow rates, grains through the entire depth of the channel were mobilised and the self-similarity ceased, with velocity profiles becoming gradually more symmetric, towards those more typical of Poiseuille flow.

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## **Reinforcing and balancing feedback loops driven by dissolution and precipitation in reactive transport through porous media**

**Author:** Andres Clarens<sup>1</sup>

<sup>1</sup> *University of Virginia*

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In order for us to use the subsurface for novel energy applications, we need a better understanding of the feedback mechanisms wherein chemical reactions accelerate or suppress transport. Applications such as geologic carbon storage, geothermal energy production, waste disposal, or energy storage all present new opportunities for transitioning to a low carbon future but all involve the injection of fluids that interact with host rocks in complex ways. Predicting the flow of fluids in chemically and physically heterogeneously rock will be important to understanding how these technologies will perform over long time scales. Here we report on efforts to measure and then model the transport of CO<sub>2</sub> and water through rock containing mineral silicates. These silicates react with CO<sub>2</sub> to form multiple products some of which can be resolubilized over time and some of which are stable. The soluble species, such as carbonate, will precipitate within pore bodies, creating a reactive front and opening flow pathways over time. The stable species, which consist largely of silicate hydrates, can block flow creating negative feedback loops that will suppress long term fluid migration. Using a suite of micro- and macroscale techniques including air permeability, scanning electron microscopy and energy dispersive X-ray spectroscopy (SEM-EDS), synchrotron  $\mu$ X-ray diffraction ( $\mu$ XRD), and synchrotron  $\mu$ X-ray fluorescence (XRF) mapping I will discuss how these processes play out in diffusion dominated column experiments conducted under reservoir conditions, high pCO<sub>2</sub>, high temperature, and buffered pH. The model system is very sensitive to initial pH conditions since dissolution processes control the leading edge of the reaction front. Interesting differences are observed experimentally between polymorphs of the same calcium silicate, which support the idea that regional dissolution processes can play an important role in controlling reactions and in turn fluid transport. After precipitation begins, the ways in which certain phases grows has an outsized impact on fluid transport. The growth of calcium silicate hydrates will be highlighted in particular because it tends to occur selectively within pore throats, which gives these reactions a disproportionately important role in limiting flow. In contrast, carbonates, which crystalize out of solution more uniformly in the pore space, are much less important in controlling fluid flow. Reactive transport modeling of this system reveals the interplay between dissolution-precipitation, volume changes, and porosity/permeability. The model incorporates microporosity in the calcium silicate phases to capture the changes observed in the experimental work and this has important implications for long term fluid transport. The modeling and its comparison with experimental work provides insight about how reactive transport modeling involving complex precipitate formation can be modeled in other contexts.

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## Relative Permeability in Reactive Carbonate Rock

**Author:** Johnathan Moore<sup>1</sup>**Co-authors:** Dustin Crandall<sup>2</sup>; Paul Holcomb<sup>3</sup><sup>1</sup> AECOM<sup>2</sup> National Energy Technology Lab<sup>3</sup> Leidos Research Support Team at the National Energy Technology Laboratory**Corresponding Authors:** johnathan.moore@netl.doe.gov, paul.holcomb@netl.doe.gov, dustin.crandall@netl.doe.gov

Geologic carbon storage at scales needed to reduce anthropogenic CO<sub>2</sub> emissions will require sequestration in numerous rock formations. The injection of CO<sub>2</sub> into carbonates has promise due to the high porosity, permeability and ubiquity of these rocks. Unlike sandstones, carbonates present a unique challenge in the form of high reactivity when exposed to the CO<sub>2</sub>-acidified brine. CO<sub>2</sub>-acidified brine, or carbonic acid, is the result of injected CO<sub>2</sub> and native brines mixing. The alteration of carbonate pore structures due to interactions with CO<sub>2</sub>-acidified brine results in a changing porosity and permeability in the formation as injections proceed. The dynamicity of the formation flow properties during injection means that readily used methodologies for parameterizing relative permeability behavior and CO<sub>2</sub> migration do not describe the system effectively.

We present a method to capture the evolution of relative permeability of a carbonate system using an unsteady-state relative permeability technique combined with computed tomography (CT) scanning. Samples were saturated with a CT-contrasting brine to simulate in-situ connate conditions within the carbonate samples, at which point absolute permeability was also determined. Supercritical CO<sub>2</sub> was then injected into the samples until residual brine saturation was achieved to determine relative permeability at a given flow rate. The sample was then re-saturated with brine to remove any residual CO<sub>2</sub>, and the newly evolved absolute permeability was measured. Intermediate CT scans taken during the flow tests were used to determine how much porosity was gained from dissolution, which was extracted from the images and utilized to calculate the new pore volume of the rock. The updated porosity and absolute permeability at each flow rate facilitated determination of new updated relative permeability curves for the sample.

The prevalence of carbonates worldwide and their favorable storage characteristics, including high porosity and permeability, make these lithologies essential in large-scale carbon storage planning. It is therefore essential to characterize how CO<sub>2</sub> flow properties evolve during active injection in carbonates. In this work, we present a methodology for characterizing relative permeability in formations where worm-hole formation and dissolution are dominant processes during CO<sub>2</sub> injection.

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MS8 / 500

## Relative contributions of permeability heterogeneity and viscosity contrast on scalar mixing

**Authors:** Alessandra Bonazzi<sup>1</sup> ; Maria Morvillo<sup>1</sup> ; Jinwoo Im<sup>1</sup> ; Birendra Jha<sup>1</sup> ; Felipe P. J. de Barros<sup>1</sup>

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Solute transport in porous media is affected by several factors. The heterogeneous structure of the permeability field is a key factor controlling the spreading and mixing behaviors of a solute cloud. On the other hand, other factors such as the viscosity contrast between the dissolved solute and the ambient fluid can also play an important role. Although both these mixing mechanisms (field heterogeneity and viscosity contrast) had been acknowledged and studied, further investigation is needed in order to better characterize the effect of the variation of both the degree of viscous fingering and the level of disorder of the porous medium. This work aims to explore the impact of field heterogeneity and viscosity contrast on the transport behavior of an inert solute in a two-dimensional flow field. To achieve this, we performed high-resolution numerical simulations to solve coupled flow and transport equations for a given range of viscosity contrast and log-permeability variance. We analyze the degree and rate of mixing, contour length of the scalar cloud, spatial statistics of the concentration field and arrival times at a control plane to characterize spreading and mixing in the domain. We provide a quantitative separation of the impacts of fingering and heterogeneity and we parameterize the concentration probability distribution function. We find that the interplay between viscous fingering, high-permeability channeling, and low-permeability stagnation at small scales create important features in the spreading and mixing characteristics.

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## Remobilization of Colloids in Porous Media Under Unsaturated Condition in column-scale experiments

**Author:** Vahid Nikpeyman<sup>1</sup>

**Co-authors:** S. Majid Hassanizadeh<sup>1</sup> ; Amir Raouf<sup>1</sup>

<sup>1</sup> *Utrecht University*

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Studies of colloid transport during transient flow in variably saturated porous media are important to determine the roles of dominant processes on particle remobilization. The main objective of this study is to develop a model to describe transport, adsorption, and release of colloids during cycles of drainage and imbibition under various saturation conditions. For this purpose, two different modelling methods were investigated. In the first set of equations, the extensions of the model of Cheng and Saires<sup>1</sup>, which was proposed by Qiulan et. al.<sup>2</sup> is examined. This model includes the empirical coefficients that quantify the kinetics of colloid mobilization during transient conditions. This formulation assumes that attachment and detachment at the air-water interface (AWI) occurs as a function of the available air-water interfacial area (a). In the second approach, we assumed that colloid exchange term from the AWI is a kinetic sorption process in which the amount of fluid saturations

determines the magnitude of air-water interfacial area. To obtain the optimized values of parameters we employed a genetic algorithm optimization scheme in both approaches. We found rather similar results between the two approaches, while slightly more accurate results were obtained using the second model. The results of simulations revealed a promising description of column scale experiments, using *Escherichia coli* D21g particles, performed by wang et al<sup>3</sup>. Numerical simulations demonstrated that the amount of colloids release is a function of the number of drainage and imbibition cycles. Furthermore, the amounts of release during the imbibition cycle was much higher than that of drainage which would be related to the important role of AWI on particle remobilization. This finding is consistent with the outcomes of experiments.

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- 1- Cheng, T., and J. E. Saiers (2009), Mobilization and transport of in situ colloids during drainage and imbibition of partially saturated sediments, *Water Resour. Res.*, 45, W08414, doi:10.1029/2008WR007494.
- 2- Zhang, Q. L., S. M. Hassanizadeh, A. Raoof, M. T. van Genuchten, and S. M. Roels (2012), Modeling virus transport and remobilization during partially saturated flow, *Vadose Zone J.*, 11, doi:10.2136/vzj2011.0090.
- 3- Wang, Y., S. A. Bradford, and J. Simunek (2014), Release of *E. coli* D21g with transients in water content, *Environ. Sci. Technol.*, 48, 9349– 9357, doi:10.1021/es501956k. **Acceptance of Terms and Conditions:**

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## Representative elementary volume for Opalinus Clay from three-dimensional pore structure and transport analysis

**Authors:** Yuankai Yang<sup>1</sup> ; Naila Ait-Mouheb<sup>1</sup> ; Jenna Poonoosamy<sup>1</sup> ; Guido Deissmann<sup>1</sup> ; Dirk Bosbach<sup>1</sup>

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Understanding the transport processes in clay rocks such as Opalinus Clay (OPA) is essential for their usage as host rocks for geological disposal of high-level radioactive wastes. The sandy facies of OPA is heterogeneous and anisotropic, comprising intercalated sandy and carbonate-rich layers in the clay rock matrix. The representative elemental volume (REV) analysis can provide an enhanced understanding between macroscale and microscale properties of a multiscale porous media. This study compares the REV for both mineral components and effective diffusivities based on two- and three-dimensional images (i.a. SEM and microCT) of the sandy OPA facies. The diffusion in the microstructures across scales is simulated by the Lattice Boltzmann Method. Our results reveal that the relationship between diffusion-based REV and component-based REV is not consistent, and the diffusion-based REV is usually smaller than component-based REV, which is also proved by our through-diffusion tests of tritiated water (HTO). The classical definition of anisotropy as a rotationally dependent parameter means that the rotation of the drill hole can also change the anisotropy of the materials. Therefore, to define a rotationally invariant anisotropy, this study provides a method to find the main directions and the main diffusivities along with the main orientations of the materials.

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## Research on pore-scale hydrate permeability prediction based on machine learning

**Author:** Ziwei Bu<sup>1</sup>

**Co-authors:** Jianchun Xu<sup>1</sup>; Hangyu Li<sup>1</sup>; Xiaopu Wang<sup>2</sup>; Shuyang Liu<sup>1</sup>

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Natural gas hydrate has huge reserves and is one of the most potential carbon energy resources. In the process of natural gas hydrate production, the phase state changes in the formation. Until now, the gas-liquid two-phase flow mechanism is not well understood for gas hydrate formation. The permeability of gas and water determines the flow capacity of fluids in hydrate formation and directly affects the efficiency of natural gas production. Since gas-water two-phase flow can cause changes of hydrate saturation and pore structure, the studies on the relative permeability is not inadequate. This study uses a combination of numerical simulation and machine learning to learn the relationship among pore statistical characteristic, the pore habits of hydrates, hydrates saturation and permeability. The goal is to reveal the seepage characteristics of hydrates at pore scale. Using COMSOL Multiphysics software, pore-scale hydrate models are established, the N-S equation is used to describe the gas-water flow. Gas-water two-phase flow are simulated. A large number of data samples are generated and the pore-scale permeability prediction database is conducted. Based on the data samples generated by COMSOL Multiphysics, machine learning algorithms are used for permeability analysis. The hydrate permeability calculation model considering different hydrate pore habits (pore filling, particle coating, et al.) , pore statistical characteristic, and saturation is established. Then, the model is verified by comparing it with the classical capillary model and Kozeny particle model. The new model provides theoretical support for flow prediction of hydrate porous media.

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## Resolving flow path resistance in heterogeneous porous media as a graph-theory problem

**Authors:** Zoe Kanavas<sup>1</sup>; Veronica Morales<sup>1</sup>; Francisco Perez-Reche<sup>2</sup>

<sup>1</sup> *University of California, Davis*

<sup>2</sup> *University of Aberdeen*

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This work aims to understand the relationship between the spatial flow distribution and its underlying pore structure in heterogeneous porous media. Thousands of two-dimensional samples of polydispersed granular media are used to 1) obtain the velocity field via direct numerical simulations, and 2) conceptualize the pore-network as a graph in each sample. Analysis of the flow field allows us to first identify the primary flow paths. Then, the graph edges are weighted by structural

attributes of the individual pores to find the shortest path through the sample. Overlap between the primary flow paths and the predicted shortest path determines the accuracy of the weighting scheme tested. A differential evolution genetic algorithm is employed to determine the “fittest” weighting scheme that maximizes accuracy while minimizing overparameterization. Our results demonstrate that the path of least resistance is accurately predicted in all samples for single phase flow and is independent of the flow distribution (uniform to preferential). The results of this work could be used for fast – relative to computationally expensive direct numerical simulations – characterization of porous media heterogeneity, which in turn can be used to predict the time of first arrival and location based on structural information alone.

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MS14 / 437

## Reversible Degradation of Diclofenac under Biotic, Denitrifying Redox Conditions: Geochemical Model and Uncertainty Quantification

**Authors:** Laura Ceresa<sup>1</sup> ; Alberto Guadagnini<sup>2</sup> ; Monica Riva<sup>2</sup> ; Giovanni Porta<sup>2</sup>

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Drinking water resources and the associated delicate aquatic ecosystem are threatened by several contaminants. A growing emphasis is nowadays given to Pharmaceuticals, such as antibiotics and analgesics. Amongst these, Diclofenac poses major concerns due to its persistent nature and frequent detection in groundwater. Despite some evidences of its biodegradability under reducing conditions, Diclofenac attenuation is often interpreted through geochemical models which are too simplified, thus potentially biasing the actual extent of its degradation. In this context, we suggest a modelling framework based on the conceptualization of the molecular mechanisms of Diclofenac biodegradation which we then embed in a stochastic context. The latter enables one to quantify predictive uncertainty. Reference environmental conditions (biotic and denitrifying) are taken from a set of batch experiments that evidence the occurrence of a reversible degradation pathway (Barbieri et al., 2012), a feature that is fully captured by our model. The latter is then calibrated through a Maximum Likelihood approach, assisted by modern sensitivity analyses. Our results fully embed uncertainty quantification and support the recalcitrance of Diclofenac in groundwater.

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Barbieri, M., Carrera, J., Ayora, C., Sanchez-Vila, X., Licha, T., Noodler, K., Osorio, V., Perez, S., Koock-Schulmeyer, M., de Alda, M.L., et al., 2012. Formation of diclofenac and sulfamethoxazole reversible transformation products in aquifer material under denitrifying conditions: batch experiments. *Science of the Total Environment* 426, 256-263. **Acceptance of Terms and Conditions:**

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MS25 / 625

## Revisiting pedotransfer function databases by fitting dual porosity model and analyzing matrix and macro-pore properties

**Authors:** Yonggen Zhang<sup>1</sup> ; Lutz Weihermüller<sup>2</sup> ; Brigitta Szabo<sup>3</sup> ; Harry Vereecken<sup>2</sup>

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Soil database was traditionally used to characterize uni-modal soil water retention curve and hydraulic conductivity curve in the past decades. However, soil is often shown to have dual-modal property, being described by macropores/fracture pore system and matrix pore system, respectively, indicating structured soils/fractured rocks and microscopic soils. Here we employed widely-used pedotransfer function databases, including UNSODA 2.0, Vereecken, and HYPRES databases, to characterize both uni-modal and dual-modal water retention curves and hydraulic conductivity curves. Only undisturbed samples were selected from the databases. We further required strict criteria to choose the soil samples to ensure that there is enough information in the measurement. A new fitting approach was then proposed to obtain the global minimal soil hydraulic parameters for both the unimodal and dual-modal Mualem van Genuchten (MvG) functions (van Genuchten, 1980; Mualem, 1976). Results suggested there is a decreasing trend of alpha (inverse of air entry parameters) and n (pore size distribution parameters) with the increasing of alpha values in the MvG functions. This trend seems to contradict our physical principles that larger alpha values usually correspond to larger n values. The decreasing trend between alpha and n were further verified analytically. We also find that the ratio of n parameters between macropore and matrix properties has an interesting relationship with the weighting factors obtained from the fitting of dual-modal soil water retention curve and hydraulic conductivity curve, respectively, for the two properties. We anticipate that the results will help to derive soil pedotransfer functions for macropore and matrix properties, which might alleviate unrealistic combinations of MvG parameters.

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Poster + / 17

## Rheology of a mixture of compressible and incompressible immiscible fluids in the capillary fiber bundle model

**Authors:** Hyejeong Cheon<sup>1</sup> ; Subhadeep Roy<sup>1</sup> ; Santanu Sinha<sup>2</sup> ; Alex Hansen<sup>3</sup>

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When capillary and viscous forces compete, there is experimental evidence for the flow velocity to depend on the pressure gradient to a power between 1.5 and 2.1. Some of these experiments are



done with both immiscible fluids being incompressible, and some are done with one of the fluids being compressible and the other being incompressible. On the other hand, the theory that has been presented on this phenomenon has assumed that the fluids being incompressible [2]. We present here a numerical and analytical investigation of the flow velocity vs. pressure drop in a capillary fiber bundle model filled with two immiscible fluids, one of which is compressible.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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MS9 / 18

## Rheology of two-phase flow in mixed-wet porous media: Dynamic network model and capillary fiber bundle results

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We expect quantitative changes in the behavior of immiscible two-phase flow in porous media when we move from uniform to mixed wet conditions 1. Are there also qualitative changes? When viscous and capillary forces -the latter determined by the wetting conditions - compete, there is growing evidence that the flow rate depends on the pressure gradient to a power in the range 1.5 to 2 [2]. These studies have all been performed under uniform wetting conditions. Do we still see this behavior under mixed wet conditions? Using a dynamic network simulator where we follow the motion of the fluid interfaces through the porous medium [3], and a capillary fiber bundle model [4], which is analytically solvable, we demonstrate that indeed we find the same qualitative behavior under these conditions [5].

#### Time Block Preference:

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MS7 / 207

## Rigorous derivation of an effective model for reactive transport in evolving porous medium

**Author:** Markus Gahn<sup>1</sup>

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<sup>1</sup> IWR, University of Heidelberg

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In this talk we derive a homogenized model for a reaction-diffusion equation describing mineral precipitation/dissolution in an evolving porous micro-domain, consisting of a fluid phase and a solid phase build by periodically distributed spherical solid grains. The evolution of the micro-domain depends on the concentration at the surface of the grains, leading to a free boundary value problem on the micro-scale. The periodicity and the size of the grains is of order  $\epsilon$ , where the parameter  $\epsilon$  is small compared to the size of the whole domain. The radius of every micro-grain depends on the concentration at its surface, leading to a nonlinear problem. The aim is to pass to the limit  $\epsilon \rightarrow 0$  and rigorously derive a macroscopic model, the solution of which approximates the solution of the microscopic model.

In a first step we transform the problem on the evolving micro-domain to a problem on a fixed periodically perforated domain by using the Hanzawa-transformation, depending on the radius of the grains and therefore the concentration. This leads to a change in the coefficients of the equations, which now depend on the radius and the concentration, leading to a nonlinear problem. We prove existence using the Rothe-method and derive *a priori* estimates for the solutions uniformly with respect to the parameter  $\epsilon$ . For the derivation of the macroscopic model in the limit  $\epsilon \rightarrow 0$  we use rigorous homogenization methods like the two-scale convergence. For the treatment of the nonlinear terms we need strong compactness results.

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## Robust porous media flow control using Deep Reinforcement Learning

**Authors:** Atish Dixit<sup>1</sup> ; Ahmed H. Elsheikh<sup>2</sup>

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With the recent progress in reinforcement learning (RL) research, we investigate whether it would be suitable to use RL in solving optimal well control problem with uncertain reservoir models. In principle, RL algorithms are capable of learning optimal action policies – a map from states to actions – to maximize a numerical reward signal. In the RL formulation of porous media flow control problems, we represent the state with snapshots of subsurface flow simulation; the action with valve openings controlling flow through sources/sinks (i.e., injection/production) wells while the numerical reward refers to the total sweep efficiency. Optimal control policies are learned by numerous episodes of simulation trials (referred to as agent-environment interactions in the RL literature).

The major challenge in learning an optimal flow control policy for well control is that the reservoir simulation often comprises of uncertain parameters (e.g., permeability fields). To the best of our knowledge, so far, such policies are learned by simply incurring samples of parameter uncertainty distribution in each episode of agent-environment interactions. Such a policy learning process is often very unstable. Furthermore, it requires a very high number of episodes, such that the variety of parameter uncertainty domain is thoroughly explored. This is computationally quite intensive for porous media flow problems for subsurface reservoir. Therefore, we investigate if we can learn the robust optimal policy with just few samples of uncertainty distribution in order to cope with these limitations.

We present two test cases representing two distinct permeability uncertainty distributions as a proof of concept for our study. Policy based model-free RL algorithms like PPO (proximal policy optimization) and A2C (advantage actor-critic) are employed to solve the robust optimal control problem for both test cases. The results are benchmarked with the optimization results obtained using differential evolution algorithm.

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## Root zone soil moisture estimation with Random Forest

**Authors:** Coleen Carranza<sup>1</sup> ; Corjan Nolet<sup>2</sup> ; Michiel Pezij<sup>3</sup> ; Martine van der Ploeg<sup>4</sup>

<sup>1</sup> *Wageningen University*

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Accurate estimates of root zone soil moisture (RZSM) at relevant spatio-temporal scales are essential for many agricultural and hydrological applications. Applications of machine learning (ML) techniques to estimate root zone soil moisture are limited compared to commonly used process-based models based on flow and transport equations in the vadose zone. However, data-driven ML techniques present unique opportunities to develop quantitative models without having assumptions on the processes operating within the system being investigated. In this study, the Random Forest (RF) ensemble learning algorithm, is tested to demonstrate the capabilities and advantages of ML

for RZSM estimation. Interpolation and extrapolation of RZSM on a daily timescale was carried out using RF over a small agricultural catchment from 2016 to 2018 using in situ measurements. Results show that RF predictions have slightly higher accuracy for interpolation and similar accuracy for extrapolation in comparison with RZSM simulated from a process-based model combined with data assimilation. RF predictions for extreme wet and dry conditions were, however, less accurate. This was inferred to be due to infrequent sampling of such conditions that led to poor learning in the trained RF model and to incomplete representation of relevant subsurface processes at the study sites in the RF covariates. Machine learning methods such as RF are promising additions to process-based models to estimate soil moisture. It offers flexibility to easily integrate various relevant datasets, such as remotely sensing imagery, in training RF models. Furthermore, these trained models can be advantageous in data-poor regions where accurate information on soil hydraulic parameters are missing or incomplete, especially when the primary goal is the estimation of soil moisture states.

Carranza, C., Nolet, C., Pezij, M., & van der Ploeg, M. (2021). Root zone soil moisture estimation with Random Forest. *Journal of hydrology*, 593, [125840]. <https://doi.org/10.1016/j.jhydrol.2020.125840>

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## Rotated Bounding Box Faster RCNN for Fracture Detection in X-Ray CT Image of Rocks

**Authors:** Ngoc Chuyen Pham<sup>1</sup> ; Changlun Sun<sup>1</sup> ; Sun Yeom<sup>1</sup> ; Li Zhuang<sup>1</sup> ; Hyu-Soung Shin<sup>1</sup>

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Quantitative evaluation of rock fracture properties including aperture, roughness and orientation is very important for rock mass characterization as the fractures properties control hydraulic and mechanical behavior of the rock. In an X-Ray CT slice, fractures are appeared as arbitrary-oriented curve-like object with low gray-scale intensity. Fracture geometry information can be obtained after manually segmentation or automatically intensity-based segmentation. In intensity-based segmentation method, curve-like enhancement filter (i.e. Hessian-based filter) is usually adopted to enhance the contrast of the fractures, which however also amplifies the edge of non-fracture objects. Therefore, fracture segmentation is still a challenging task. To overcome this difficulty, we propose to use oriented bounding boxes as the basis anchor of the Faster RCNN algorithm to automatically detect fractures in CT images. In comparison with axis-aligned bounding box, the rotated bounding box significantly improves the ratio of object-of-interest to background within the bounding box and also handles arbitrary-oriented elongated objects more effectively. The primary result shows that rotated bounding box outperforms axis-aligned bounding box in the fracture detection task. Furthermore, different segmentation schemes including Hessian-based filter, U-Net and segmentation branch like Mask RCNN will be investigated and compared in order to determine the most effective method for fracture segmentation within the detected bounding box.

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## **SIMULATION STUDY OF IN-SITU CONVERSION PROCESS IN LOW-MID MATURITY SHALE OIL RESERVOIR**

**Authors:** Zijie Wang<sup>1</sup> ; Jun Yao<sup>None</sup> ; Hai Sun<sup>1</sup> ; Lijun Liu<sup>1</sup> ; Xia Yan<sup>None</sup>

<sup>1</sup> *China University of Petroleum (East China)*

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Continental shale oil in China is mainly of low-medium maturity. The formation is filled with heavy oil of low mobility and organic matter that unconverted. Horizontal drilling and hydraulic fracturing are insufficient to obtain economic production in such reservoir, thus in-situ heating and transform technology should be applied. To describe the decomposition of solid organic matter, cracking of heavy hydrocarbon, phase behavior and composition evolution, we developed a multiphase multi-component hydro-thermal coupled numerical model and numerical solution method by considering multistage kinetic reactions. Then the impact of parameters including heating temperature, kerogen concentration, well bottom hole pressure, heating space and initial water saturation on cumulative production is analyzed. The results are summarized as: kinetic reaction rate is controlled by temperature and different reactions take place at variety heating temperature; higher kerogen concentration can enhance cumulative hydrocarbon production after in-situ conversion; low bottom hole can extract oil and gas quickly to prevent from coking; larger heating spacing would weaken the effect of in-situ conversion process, while the product will further crack with too small heating spacing; high water saturation will enhance energy consumption to heat water and reduce the utility ratio of energy, thus dewater process is required to reduce water saturation. This study analyzed shale oil in-situ conversion process based on thermal-reactive flow. The model developed can be used to evaluate the heating process and provide theoretical support for the efficient development of shale oil reservoir.

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MS8 / 654

## **Saturated Colloid transport experiments under unfavorable conditions in Dual-Porosity PDMS micro-models.**

**Authors:** Enno de Vries<sup>1</sup> ; Amir Raof<sup>1</sup> ; Qianjing Tang<sup>1</sup>

<sup>1</sup> *Utrecht University*

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Increased use of natural and engineered colloids and nanoparticles in agriculture, industry, and consumer products leads to more exposure of these particles to soils. Transport of particles through the subsurface attracted attention since they are being detected in the environment in larger amount and also in our nation drinking water supplies which can pose health threat. Preferential flow caused by aggregated soil profiles, or porous media that are structured, fractured, or microporous in other ways can be a mayor contributor to surface and subsurface pollution problems.

In this study we manufactured PDMS micromodels based on x-ray tomography and transformed solid grains into aggregates. We replaced 25, 50, 75, and 100% of the solid grains into aggregates. The models have distinct inter-aggregate and intra-aggregate pores. We explored colloid transport under unfavorable conditions by improving three major shortcomings: domain size, imaging resolution and frame rate. We have developed an optic set-up allowing for imaging with a high resolution of 2.9  $\mu\text{m}$ , applying large micromodel with length and width of 10 millimeter with unstructured design, and a frame rate of 10 frames per second. We have captured the full trajectory of a large number of colloids flowing through pore structures at the same time and capturing their dynamics under unfavorable conditions in the presence of a high energy barrier. Streamline of each colloid within the domain was obtained and further divided into three categories of fully mobile, full attached, and remobilized particles which were analyzed in detail. We have used 4 micrometer colloids and applied an average velocity of 50 cm/hr.

During all experiments over 1500 colloid trajectories were observed. While chemical conditions is unchanged between the samples a high increase from almost 0 % with no aggregates present to 40% of colloid retention with 100% of aggregates. Remobilization events were rare in all models. The trajectory tortuosity decreased from 1.21 to 1.15 due to the increased amount of aggregates leading to shorter flow paths. By introducing aggregates there is a much higher chance for colloids to be transported through the intra-aggregate pores leading into a higher chance for the colloid to interact with a collector surface and attach, adding as well the lower flow velocities inside them attribute to attachment.

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## Scalable Multilevel Methods for Poroelasticity

**Author:** Arne Nägel<sup>1</sup>

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Developing efficient solvers for coupled PDE systems is often a non-trivial task, since one must combine suitable schemes for time integration and linear solvers. In this study, we suggest a combination of methods for the quasi-static Biot system, which scales on nowadays's HPC systems.

One classic approach is the fixed stress iteration, e.g. (Kim et al., 2011). This be interpreted as a special block-LU decomposition for the coupled system, where degrees of freedom for deformations and pressures are separated. It is a key observation that the Schur complement, when formed w.r.t the pressure, can be approximated by a properly scaled identity (e.g., Mikelic and Wheeler, 2013). The method can be generalized to deal with jumping coefficients in heterogeneous media (e.g., Both et al., 2017).

In this work, we avoid the aforementioned splitting and employ a multigrid solver for the fully-coupled system. The method is based on the fixed-stress smoothers suggested by (Gaspar und Rodrigo, 2017). We investigate its robustness for heterogeneous media and provide a scaling study in an HPC environment. Our numerical experiments also include a combination with linearly-implicit extrapolation schemes which allow for an adaptive time-stepping.

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## Scaling and errors estimates of the effective Brinkman viscosity

**Authors:** Shervin Bagheri<sup>1</sup> ; Ugis Lacis<sup>2</sup> ; Aidan Rinehart<sup>3</sup>

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We investigate the Brinkman equation for modelling free flows over porous media. Using scaling estimates we show that the Brinkman viscosity  $\mu_b$  satisfies

$$\begin{equation} \mu_b = C \mu \frac{\ell_s^2}{k}, \end{equation}$$

where  $\mu$  is molecular viscosity of the fluid,  $C$  is a constant of order one,  $k$  is a measure of the permeability tensor and  $\ell_s$  is the Navier slip length at the interface plane between the porous medium and the free flow. Using pore-scale direct numerical simulations of shear and pressure driven flows over a range of both regular and irregular porous materials, we confirm the scaling relation above for porous surfaces that form a rough interface with the overlying flow. We also assess the errors of using the Brinkman equation to model the interaction between free flows and porous materials. We find that the errors peak to large values ( $\sim 30\%$  in the 2-norm) around solid volume fractions  $\Phi = 10^{-2}$ . We explain physically these errors and discuss the appropriateness of using the Brinkman equation to model free flows over porous media.

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MS21 / 679

## Scaling of vertical mixing in two-species buoyancy-driven instabilities

**Authors:** Anne De Wit<sup>1</sup> ; Shyam Sunder Gopalakrishnan<sup>1</sup> ; Bernard Knaepen<sup>1</sup>

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A miscible horizontal interface separating two solutions of different solutes can deform into convective finger-like structures due to buoyancy-driven instabilities like the classical Rayleigh-Taylor instability or the double-diffusive instabilities, triggered by differential diffusion of the solutes in the solutions. We analyse numerically for porous media flows the scaling of the fingers vertical speed, defined as the slope of the temporal

evolution of the mixing length of the fingers. In the parameter space of the problem, spanned by the buoyancy ratio  $R$ , and the ratio  $\delta$  of diffusion coefficients of the two species, the vertical speed is found to scale linearly with the adverse density difference that drives the convective mixing in these flows. The adverse density difference is the density jump across the spatial domain where the density gradient of the diffusive base-state is negative along the direction of gravity. It can be computed analytically from the diffusive base-state density profile and can be significantly different from the initial density difference when differential diffusion of the solutes are at play. Our results evidence the possibility of controlling the nonlinear evolution of mixing of buoyancy-driven instabilities in two-species stratifications

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## Self-assembly of *Comamonas denitrificans*: formation of a living bacterial gel

**Author:** Sam Charlton<sup>1</sup>

**Co-authors:** Eleonora Secchi<sup>2</sup> ; Gavin Melaugh<sup>3</sup>

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Bacterial autoaggregation is a phenomena widely exhibited by environmental and pathogenic bacterial species [1]. Autoaggregation is mediated through surface bound and secreted proteins and polysaccharides and can act as a precursor to surface bound biofilm formation. Aggregation is considered a survival strategy, commonly induced by unfavourable growth conditions and low metabolic activity [2]. Polymer bridging and depletion attraction have been demonstrated to trigger autoaggregation, typically forming structures of compact disconnected clusters [4, 5].

*Comamonas denitrificans* is a rod shaped filamentous bacterium found in abundance in wastewater environments which displays highly efficient denitrifying capabilities and exoelectrogenic activity in microbial fuel cells [6, 7, 8]. Our studies with this bacterium revealed autoaggregation which displays a distinct gelation phase transition at intermediate volume fractions ( $\phi > 0.008$ ). In this work we apply multiscale techniques from the soft matter toolbox to investigate the aggregation kinetics of *Comamonas denitrificans*. For the first time we show that bacterial autoaggregation can lead to self-assembly of space spanning fractal networks akin to attractive colloidal gels. By altering dissolved oxygen conditions during cell culture, we are able to reliably tune cell aspect ratio distribution and gel porosity creating a controllable living colloidal system. Using optical microscopy, we study the aggregation dynamics of low and high aspect ratio distributions, in the presence and absence of bacterial growth and in density matched and mismatched conditions. We compare the bacterial gel dynamics against Brownian dynamics simulations to further access the impact of aspect ratio distribution on the bacterial gel connectivity and porosity, and consider the impact of uniform or polar bonding locations. This work is a first look into self-assembled bacterial 'living gels'.

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## Self-sealing in wellbore cement under CGUS conditions by micro-CT, SEM, DM, and Raman

**Authors:** Yan WANG<sup>None</sup> ; Liwei Zhang<sup>1</sup> ; Manguang Gan<sup>None</sup>

<sup>1</sup> *Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

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In this study, reaction experiments between CO<sub>2</sub>-saturated brine and wellbore cement samples cured under different pressures were conducted to study microstructural and mineral composition changes using micro-computed tomography (micro-CT), scanning electron microscopy (SEM), digital microscope (DM) and Raman spectroscopy. The CT images of post-CO<sub>2</sub> exposure cement samples showed a dissolution-precipitation-dissolution pattern at the exterior of the samples. The dissolution in the inner borehole of the samples, however, was not significant. Instead, only CaCO<sub>3</sub> precipitation was observed in the inner borehole. CaCO<sub>3</sub> precipitation in the inner borehole contributes to self-sealing of the cement, which reduces the risk of CO<sub>2</sub> leakage through wellbore cement. According to CT and SEM observations, a higher curing pressure caused more precipitation of CaCO<sub>3</sub>, which favored cement self-sealing when exposed to CO<sub>2</sub>. The appearance of C=O a peak and the disappearance of -OH peak after reaction with CO<sub>2</sub> were observed by Raman spectroscopy, which was attributed to cement carbonation that converted Ca(OH)<sub>2</sub> into CaCO<sub>3</sub>. This study provides solid evidence of cement self-sealing due to cement carbonation under geologic CO<sub>2</sub> storage circumstances.

Keywords

Wellbore cement; self-sealing; CO<sub>2</sub> storage; CT scanning; carbonation

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## Semantic segmentation of microCT and FIB-SEM rock images using deep learning methods

**Authors:** Jack Ringer<sup>1</sup> ; Hongkyu Yoon<sup>1</sup>

<sup>1</sup> Sandia National Laboratories

**Corresponding Authors:** hyoon@sandia.gov, jringer@sandia.gov

Recent advances in multiscale imaging techniques for the analysis of complex pore structures and compositions have revolutionized our ability to characterize various porous media systems. Segmentation of images obtained from different image techniques such as X-ray computed microtomography ( $\mu$ CT) and scanning electron microscopy (SEM) is the first step to quantitatively describe various features of geomaterials. However, conventional methods such as thresholding, watershed segmentation, and other predefined algorithms are subject to user bias, often require specific segmentation processes for each image set, and can fail to adapt to certain datasets. In this work we evaluate the capability of convolutional neural networks (CNNs)-based algorithms to segment both  $\mu$ CT and focused ion beam-SEM (FIB-SEM) images with varying degree of challenges for image segmentation. The performance of three different 2D CNN architectures (VGG16, ResNet, and U-Net) as well as a few 3D CNN architectures (U-Net and MultiResU-Net) is assessed on four independent datasets including sandstone, carbonate chalks, and shale. Each of these datasets is composed of three-dimensional image stacks and corresponding ground truth labels that were constructed with various image processing algorithms. Our results indicate that deep learning architectures can successfully be applied to the task of semantic segmentation for  $\mu$ CT and FIB-SEM images and perform better than manual segmentation to recover natural morphology of original images. In addition, our results indicate that transfer learning can allow for models to converge more quickly during training and that generic image features (learned from a large dataset such as ImageNet) can be applied to improve model performance in some cases. Performance comparison among different CNN architectures highlights the linkage of classification outcomes to underlying features of each CNN architecture and hyperparameters.

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## Separation of colloidal particles in microchannels using diffusio-phoresis

**Author:** Mamta Jotkar<sup>1</sup>

**Co-author:** Luis Cueto-Felgueroso<sup>2</sup>

<sup>1</sup> Universidad Politécnica de Madrid

<sup>2</sup> Universidad Politecnica de Madrid

**Corresponding Authors:** mamta.jotkar@upm.es, luis.cueto@upm.es

Flows containing suspended colloidal particles and dissolved solutes can occur in a variety of natural and engineered scenarios. With an objective of designing technological applications including effective separation techniques, it is desirable to gain control over the particle dynamics. Diffusio-phoresis or the chemotactic migration of colloidal particles due to local chemical gradients was first demonstrated by Derjaguin in the 1940s and later developed by Anderson & Prieve in the 1980s. In the recent years, this mechanism has received a renewed interest for achieving rapid focusing and trapping of particles. Following this motivation, we numerically study the combined effect of fluid advection and particle diffusio-phoresis driven by a local solute concentration gradient to achieve controlled trapping of the suspended colloidal particles in microchannels. More precisely, we vary the

size and surface charge of the particles to show that size-dependent and surface-charge-dependent particle separation can be achieved rapidly in dilute solutions by imposing a solute gradient. We also investigate a related phenomenon referred to as diffusioosmosis that causes bulk flow adjacent to a stationary surface, by varying the surface charge of the microchannel geometry.

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## Shale microstructures: Experimental and fractal characterization

**Authors:** Zhenhua Tian<sup>1</sup> ; Jianchao Cai<sup>1</sup> ; Wei Wei<sup>1</sup> ; Yuxuan Xia<sup>1</sup> ; Yihua Xiong<sup>1</sup><sup>1</sup> *China University of Geosciences, Wuhan***Corresponding Authors:** tianzh@cug.edu.cn, weiwei@cug.edu.cn, xiayx@cug.edu.cn, lingkongdaxia@163.com, caijc@cug.edu.cn

The microstructures of shale gas reservoirs are significant for the study of gas transport mechanisms and the formulating of the gas exploitation plan. In this work, the composition, scanning electron microscopy images, and adsorption information of Longmaxi shale samples are experimentally obtained. The fractal features of shale microstructures are systematically analyzed based on fractal theory. The correlation analyses are widely conducted among the microstructures of shale. The results show that the microfractures, intergranular pores, intragranular pores, dissolved pores, and organic pores make up the complex pore network of shale. For the studied Longmaxi shales, the adsorption isotherm is type IV and the hysteresis loop is type H3. The total organic carbon content of shale has some influences on the adsorption capacity and nanopore distribution positively. The surface fractal dimensions in the van der Waals force regime and the capillary condensation regimes are close for the marine shales evaluated, which is quite different from the two-section characteristic of continental and marine-continental shales. The statistical self-similar property of shales studied is further confirmed according to the analytical fractal equation. The large differences among the pore fractal dimensions manifest the strong heterogeneity of pore distribution of shale. Moreover, the heterogeneity of pore distribution can be quantitatively represented by the normalized lacunarity. Some universal correlations among the microstructures are found and logically explained for the shales evaluated.

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## Shear Displacements of an Embedded Fracture Network using XFVM – a Sensitivity Analysis

**Author:** Giulia Conti<sup>1</sup>

**Co-authors:** Rajdeep Deb ; Stephan Matthai <sup>2</sup> ; Patrick Jenny

<sup>1</sup> *ETH Zurich, Institute of Fluid Dynamics*

<sup>2</sup> *The University of Melbourne*

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Understanding deformation and fluid flow in a fractured rock mass is of central importance for geothermal energy extraction, wastewater disposal, and hydrocarbon exploration. Thermal strain- or fluid pressure - induced shear displacements in the fracture system lead to hydraulic aperture changes that affect the flow field. To predict these, numerical frameworks are needed that can accurately and efficiently capture this coupled mechanical and hydraulic behavior even in complex natural fractured reservoirs. For this purpose, we use the extended finite volume method (XFVM). In XFVM, the flow and mechanics solvers are iteratively coupled with the fixed stress method, modelling fractures in a poroelastic damaged rock matrix. Fractures are represented as embedded lower dimensional manifolds. The displacement of individual fractures and fracture manifolds is resolved by discontinuous basis functions, modeling slip and tensile displacements as piecewise constant on each fracture segment. Traction, including compressive forces are calculated for each fracture segment and failure criteria are evaluated.

Here we apply the described framework to analyse shear displacements in a natural fracture network under *in situ* conditions. The selected fracture pattern consists of approximately 200 non-systematic fractures mapped at Dounreay in Scotland. In a grid convergence study we investigate which grid resolution is needed to accurately resolve the stress field in the damaged rock matrix as well as the shear slip of the embedded fractures. The sensitivity of shear displacements to fracture characteristics such as for length, orientation or abutting relationships is studied.

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MS25 / 126

## **Simple models of soil hydraulic properties in the complete moisture range: Testing the new PDI model system with a comprehensive experimental dataset**

**Authors:** Wolfgang Durner<sup>1</sup> ; Tobias Hohenbrink<sup>1</sup> ; Sascha C. Iden<sup>1</sup> ; Andre Peters<sup>1</sup>

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Simulation of water, solute, and energy transport in the vadose zone requires appropriate soil hydraulic properties models. The established models implicitly assume that water storage and water flow occur only in completely filled soil pores, but neglect the so called non-capillary water (i.e. water in films on grain surfaces, and in pore corners). These models are therefore suitable to model water flow and solute transport in the medium to wet moisture range, but likely fail when soils become dry. During the last decade, modelling approaches have been developed that take into account non-capillary water. One of these is the PDI model system developed by Peters (2013, 2014) and Iden and Durner (2014). It is a simple parametric system that extends any basic model of capillary retention and conductivity with a non-capillary counterpart, requiring an additional fitting parameter for the non-capillary liquid conductivity. Despite the simple model structure, the resulting soil hydraulic curves are in close agreement with the more comprehensive physically based film flow conductivity model of Lebeau and Konrad (2010). In this paper, we (i) present a PDI model variant that replaces

the additional fitting parameter for non-capillary conductivity with a physically derived parameter, thus eliminating the need for additional fitting parameters compared to the established models, and (ii) conduct a comprehensive model performance test of several established capillary models alone (no PDI) and in combination with the original PDI, and the new PDI variant.

The model performance test is based on highly resolved water retention and conductivity data measured at 500 undisturbed soil samples. Soil water retention and conductivity data in the wet range were obtained in the laboratory by the evaporation method. Retention data in the dry range were obtained by the dew point method. For each data set we estimated the soil hydraulic parameters for nine scenarios, resulting from combinations of three basic models [ (i) van Genuchten with  $m=1-1/n$ , (ii) van Genuchten with a free parameter  $m$  (van Genuchten, 1980), (iii) Fredlund & Xing (1994)] with three considerations of non-capillary water [ (i) not considered, (ii) original PDI with additional fitting parameter for non-capillary conductivity, and (iii) the new PDI without additional fitting parameter).

The most flexible basic functions generally yielded the best model fits. Considering non-capillary water by the PDI model system clearly increased the model performance. The description of the measured retention and the conductivity data was improved in the order from original, to PDI without additional fitting parameter, to PDI with fitted non-capillary conductivity parameter. Notably, the new PDI model variant with exactly the same free parameters described data significantly better than the original models.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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## Simulating solute transport through saturated heterogeneous medium using triple porosity non equilibrium model

**Author:** Aman Chandel<sup>1</sup>

**Co-author:** Deepak Swami<sup>2</sup>

<sup>1</sup> Research scholar, School of Engineering, Indian Institute of Technology Mandi, Mandi, India

<sup>2</sup> Assistant Professor, School of Engineering, Indian Institute of Technology Mandi, Mandi, India

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This study assumes complex saturated liquid phase volume to be a triple porosity medium consisting of macro, meso and micropore structure. This provides the Triple Porosity Non-Equilibrium (TPNE) model a higher capability of mimicking the physical and chemical non equilibrium present as per the

field conditions. The method of finite difference for discretisation is used to solve the model. Semi-analytical solution of Dual Advection Dispersion Equation (DADE) (Leij et al. 2012) validates the model. Different unknown parameters are estimated using parameter estimation algorithm (PEST) and detailed sensitivity analysis is performed to delineate the behaviour of the model against various parameters. The behaviour of the model is studied for the wide range of Peclet number and Damköhler number with the help of temporal moments. The dataset from the experiments conducted on a heterogeneous soil column by Huang et al., (1995) is used to calibrate the model and is compared with Mobile Immobile (MIM) model by van Genuchten & Wierenga, (1976b). TPNE emerges as better performer capturing the early breakthrough and skewed breakthrough curves (BTC).

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Leij, F. J., Toride, N., Field, M. S., & Sciortino, A. (2012). Solute transport in dual-permeability porous media. *Water Resources Research*, 48(4), 1–13. <https://doi.org/10.1029/2011WR011502>

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MS17 / 572

## Simulation of Thermochemical Heat Storage in the CaO/Ca(OH)<sub>2</sub>-System on the Micro-Scale

**Author:** Torben Prill<sup>1</sup>

**Co-authors:** Marc Philipp Linder<sup>1</sup>; Thomas Jahnke<sup>1</sup>

<sup>1</sup> German Aerospace Center (DLR)

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Storing energy in the form of heat has been under long-standing investigation for prospective applications, such as the capturing of excess heat from industrial processes as well as storing energy in concentrated solar power plants. Investigated mechanisms for the heat storage include the adsorption in porous media, materials undergoing phase changes and thermochemical reactions. Among these, thermochemical heat storage provides a large energy capacity and next to perfect reversibility. More specifically, storage in the CaO/Ca(OH)<sub>2</sub>-System is investigated because of the low price and environmental friendliness of the reactants. In the project THEMSE, DLR is developing models and simulations for thermochemical heat storage in the CaO/Ca(OH)<sub>2</sub>-System on the microscopic level. In this talk, we shall give an overview over the project and the materials involved.

The geometrical micro-scale characterization of the material is done using a combination of micro computed tomography (μCT) and scanning electron microscopy (SEM). Both methods are complementary in the sense that SEM can be used to resolve fine scale details, up to crystallites, while μCT can resolve powder particles as well as agglomerates of numerous single particles. This is complemented by kinetics measured by thermogravimetric analysis (TGA).

The first goal in the project is to explain the measured kinetics using a spatially resolved model, which takes the three-dimensional morphology of the storage material into account. In general, this involves, thermal, hydrodynamic, mechanical, and chemical modeling. However, the first investigations involve a single crystallite model, where the thermal and hydrodynamic effects can be neglected, and which is solved using finite element simulations. Further models are developed to

investigate the heat and mass transport in the powder bed inside the reactor. Heat transport being the limiting factor, modeling the thermal conductivity of the powder bed on the microscale, is given special attention. This is done, the using simulations based on  $\mu$ CT-Data. Finally, it is investigated how the cycling of the material influences the heat and mass transport in the powder bed inside the reactor. This happens through agglomeration of powder particles the cause of which, and the modeling of which, are under investigation and under development, respectively.

We will show results from experiments and from kinetic and micro-scale transport simulations. Finally, an outlook will be given on the upscaling of the micro scale model to the reactor-scale and computational optimization methods for reactor design.

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MS20 / 671

## Simulation of blood flow in a whole mouse brain vasculature

**Authors:** Erlend Hodneland<sup>1</sup> ; Jan Martin Nordbotten<sup>2</sup> ; Noeska Smit<sup>2</sup>

<sup>1</sup> *NORCE Norwegian Research Centre*

<sup>2</sup> *University of Bergen*

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Quantification of the full brain structural vasculature and physiological response is advantageous for improved understanding of cerebrovascular disease progression affecting the brain. In this respect, characterization of the whole brain angioarchitecture across multiple resolution scales from arteries and veins down to capillaries enables simulation of whole brain blood flow. In the current work we are pioneering a blood flow simulator for a complete in silico mouse brain model previously segmented for vasculature. We report structural and functional parameters of the mouse brain angioarchitecture that to date have not been reported elsewhere.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Erlend Hodneland, Erik A. Hanson, Ove Sævareid, Geir Nævdal, Arvid Lundervold, Veronika Solteszova, Antonella Z. Munthe-Kaas, Andreas Deistung, Jurgen R. Reichenbach, Jan M. Nordbotten. "A new framework for assessing subject-specific whole brain circulation and perfusion using MRI-based measurements and a multi-scale continuous flow model". *PLOS Computational Biology* (2019); 15(6):e1007073.

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MS7 / 186

## Simulation of fractured porous media using partitioned black-box methods

**Authors:** Alexander Jaust<sup>1</sup> ; Patrick Schmidt<sup>1</sup> ; Holger Steeb<sup>2</sup> ; Miriam Mehl<sup>1</sup>

<sup>1</sup> *University of Stuttgart*

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The simulation of coupled fracture flow and deforming porous medium is a challenging problem in reservoir engineering. Common examples are hydraulic simulations or hydro-fracking. Some of the challenges arise due to the difference in properties of the mathematical models used in each of the subdomains. Solving the problem using a monolithic approach leads to an ill-conditioned system of equations implying the necessity of using a direct solver for the resulting linear system of equations.

We investigate a partitioned black-box coupling approach based on the idea of domain decomposition techniques. The individual problems are solved separately in an iterative manner such that we can use standard iterative solvers for the linear systems. Our approach is based on the open-source library preCICE ([www.precice.org](http://www.precice.org)) allowing us to reuse existing solver software and simplifying the setup of new solvers that are immediately prepared for high-performance parallel computations.

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MS25 / 720

## Soil Moisture Data Fusion from Field Scale to Continental Scale

**Authors:** Binayak Mohanty<sup>1</sup> ; Dhruva Kathuria<sup>1</sup>

<sup>1</sup> *Texas A&M University*

**Corresponding Authors:** kathuria.dhruva@gmail.com, bmohanty@tamu.edu

In past 3 decades, Harry Vereecken has addressed a number of topics related to soil hydrology covering a range of scales from pore to catchment. To honor his outstanding efforts, here we present a new data fusion scheme to merge soil moisture from various insitu and satellite platforms. In this work, we develop a novel multi-scale geostatistical algorithm which can combine massive remote sensing datasets at different spatio-temporal resolutions for enhanced understanding of the underlying physical processes. We apply the proposed algorithm combining soil moisture data from Soil Moisture Active Passive (SMAP) and Soil Moisture and Ocean Salinity (SMOS) with point data from U.S Climate Reference Network (USCRN) and Soil Climate Analysis Network (SCAN) across Contiguous US (CONUS) uncovering novel insights into soil moisture dynamics across scales. Using an underlying covariate-driven spatio-temporal process, the effect of dynamic and static physical controls—vegetation, rainfall, soil texture and topography—on soil moisture is quantified. We find that vegetation, rainfall and topography affect the mean soil moisture distribution across CONUS while soil texture determines the spatio-temporal covariance between soil moisture pixels. We successfully forecast 5-day soil moisture across CONUS for multiple spatio-temporal scales accompanied by uncertainty metrics. Finally, we discuss the potential applicability of the algorithm to future soil moisture missions and broader Earth-System processes.

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## Solute Transport in Heterogeneous Soils from Different Land Management Practices

**Authors:** Mackenzie Dughi<sup>1</sup> ; Federico Zabaleta<sup>1</sup> ; Fabian Bombardelli<sup>1</sup> ; Veronica Morales<sup>1</sup>

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The fate and transport of agrochemicals in soils have important implications for groundwater quality and public health. Land management practices deliberately change the pore structure, which consequently controls how mass is transported through the subsurface of agricultural lands. This study employs direct numerical simulations (DNS) to investigate the differences in transport behavior in porous media sampled from a long-term agricultural research station. Millimeter-size samples of soils characterized as ploughed and no tillage are analyzed. The velocity field in each soil domain is solved from the full Navier-Stokes equations and massless particle tracers are tracked accordingly. A statistical analysis of the Lagrangian tracks is presented to compare the velocity variability, breakthrough curve and evolution of displacement moments that characterize each land management practice. Statistical rules for particle motion at the pore-scale are then applied to parameterize an upscaled transport model based on Continuous Time Random Walk theory. Such a modeling framework shows promise in capturing the non-Fickian behavior that is ubiquitous in all heterogeneous media. An improved understanding of the controls for contaminant transport in agricultural soils and of the predictive tools to model contaminant transport are key to helping decision makers implement sustainable strategies in agriculture.

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## Solute transport during unstable infiltration into layered heterogeneous porous media

**Authors:** Pedro Pampillon Alonso de Velasco<sup>1</sup> ; Luis Cueto-Felgueroso<sup>2</sup> ; Ruben Juanes<sup>3</sup>

<sup>1</sup> *Universidad Politécnica de Madrid*

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**Corresponding Authors:** luis.cueto@upm.es, juanes@mit.edu, pedropampillonalonso@gmail.com

Gravity-driven infiltration of fluids into heterogeneous soil controls the distribution of water in soil and the fate and transport of pollutants through the vadose zone. Infiltration into dry soil is hydrodynamically unstable, leading to preferential flow through narrow wet regions. These preferential channels concentrate water and solute fluxes and persist over cycles of wetting and drying.

In this work, we use numerical simulation to explore the impact of fingering and layered soil structure on solute transport in the vadose zone. We validate our unsaturated flow model by reproducing experimental results of infiltration of water into various configurations of layered soil. Our model can accurately reproduce the flow behavior at the transition between layers with contrasting grain sizes. We propose to calibrate our continuum unsaturated flow model using the changes in finger width as a function of infiltrating flux and grain size contrast between layers. We simulate the transport of a passive tracer through initially dry soil and after multiple infiltration cycles, and characterize the transport mechanisms in 2D and 3D layered soils.

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MS17 / 310

## Soret effects in porous media

**Author:** Bjørn Hafskjold<sup>1</sup>

**Co-authors:** Signe Kjelstrup<sup>2</sup>; Olav Galteland; Dick Bedeaux<sup>3</sup>

<sup>1</sup> *Norwegian University of Science and Technology*

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Thermal diffusion, the Ludwig – Soret effect, plays an important role in transport of heat and mass in fluid mixtures. The coupling between heat- and mass transport extends Fourier’s law for heat conduction and Fick’s law for mass diffusion and is quantified by the Soret coefficient. The effect has applications in industrial processes, such as utilization of waste heat [1], analyses of composition gradients in oil reservoirs [2], as well as novel use in nanomachines [3]. Many experimental techniques have been used to measure Soret coefficients in bulk fluids [4]. It is known that a porous medium may have an impact on the Soret effect, but experimental data are not conclusive on its origin. For instance, porosity, permeability, wettability, and tortuosity will all change diffusion relative to bulk fluid, but the magnitude and mechanism of the coupling of mass diffusion and thermal diffusion is still unknown.

We will present results from non-equilibrium molecular dynamics simulations [5] of the Soret effect for a Lennard-Jones model with two miscible fluid components in a porous medium. The medium has different porosity and wettability preferences for the two fluid components. We show that the wettability preferences change the Soret coefficient and discuss the mechanisms that lead to such change.

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Time Block A (09:00-12:00 CET) **References:**

[1] L. Keulen, L.V. van der Ham, J. Haanemaijer, N.J.M. Kuipers, Thijs Vlugt, S. Kjelstrup, «Membrane distillation against a pressure difference», *J. Membr. Science*, 524 (2017) 151-162.

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MS10 / 561

## Spontaneous imbibition dynamics in yarns and knit stitches by fast X-ray tomography and free energy analysis

**Authors:** Robert Fischer<sup>1</sup> ; Christian M. Schlepütz<sup>2</sup> ; René M. Rossi<sup>3</sup> ; Dominique Derome<sup>4</sup> ; Jan Carmeliet<sup>5</sup>

<sup>1</sup> *ETHZ, Empa*

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Moisture management in textiles is not only of importance for functional clothing, but also for medical fabrics. Understanding or even predicting the dynamics of spontaneous imbibition in textiles is challenging due to the heterogeneity of textile structures and thus the complexity of the fiber/water/air interfaces. The physics on the pore scale determine the macroscopic water transport. Contrary to some classes of porous media, e.g. sedimentary rock, step-wise uptake/imbibition dynamics have been observed for textiles and models in the style of Darcy's or Washburn's laws cannot always be applied. We employ time-resolved X-ray tomographic microscopy (XTM) to study pore-scale filling processes and their impact on the overall imbibition dynamics.

Textiles are multiscale materials. Yarns are processed into fabrics, e.g. by weaving or knitting. The yarns are twisted bundles of fibers. The fibers can be porous themselves, but we focus in this study on dense fibers of polyethylene terephthalate (PET, not swelling) with uniform wettability and contact angle 48°. 32 continuous PET fibers with circular cross section and a diameter of 55 µm are manually spun to yarns with 200 twists per meter and mounted at given tension (2.5, 10 and 30 mN/tex) in a sample holder attached to a reservoir. The setup is placed on the rotating sample stage of the TOM-CAT beamline for synchrotron XTM at the SLS, Paul Scherrer Institut, Villigen PSI, Switzerland. By remotely filling the reservoir, we image the full spontaneous water imbibition process in a 5 mm yarn segment from an unlimited reservoir in 4D with 2.75 µm voxel size and up to one tomographic scan per second. In a second experiment, equally prepared yarns are mounted in a configuration mimicking the contact of two yarns in the wale direction of a knit stitch. This configuration forces the water to pass the yarn contact to reach the top of the field of view.

XTM reveals the inter-fiber pore system and the dynamic evolution of the water configuration with its corresponding change in free energy. The imbibition process displays two very distinct time scales. While pores are filled in quick bursts, there are long periods of almost flow stagnation at pore transitions. It is found that these periods correspond to quasi-equilibria of the water configuration with almost vanishing free energy gradient. The water reconfigures slowly until it reaches again a state with high free energy gradient that allows higher fluxes. Such high fluxes are supported by the longitudinal aspect ratio of the pores. Since these low-energy-gradient periods can last up to minutes, the overall water uptake in yarns is not dominated by the wetting speed, but by the periods when water is (almost) not flowing. Since the fiber configuration at the yarn contact prevents the formation of continuous cross-yarn pores, this yarn contact is the locus of many such slow water reconfigurations. Consequently, water uptake in both studied systems, namely single yarns and stitches, is characterized by two-scale step-wise dynamics with slowdowns at pore-to-pore and yarn-to-yarn transitions, a crucial information for potential modeling approaches of textiles.

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**Stability and performance of emulsion in bulk-scale and pore-Scale****Authors:** Mohammad Javad Shojaei<sup>1</sup> ; Senyou An<sup>2</sup> ; Vahid.J Niasar<sup>None</sup><sup>1</sup> *Imperial College London*<sup>2</sup> *University of Manchester***Corresponding Authors:** vahid.niasar@manchester.ac.uk, m.shojaei@imperial.ac.uk, senyou.an@manchester.ac.uk

Understanding emulsions' behaviour is essential for many industrial applications such as environmental remediation, Enhanced Oil Recovery (EOR), and food processing. Although several experimental studies have been previously performed to study emulsion behaviour, fewer of them have specifically addressed the correlation between emulsion behaviour in bulk-scale to pore-scale. Firstly, we tried different methods presented in the literature for making emulsions. Our findings suggest all the methods are not successful in making emulsions, and there is a specific shear rate needed to be passed for making emulsions. Then, we performed bottle test experiments to find the optimum salinity for making stable emulsion. The rheology of emulsion at bulk-scale was measured using Anton Paar Rheometer and the results compared with the rheology obtained in pore-scale using micro-models. Also, in-situ emulsion generation inside the porous media practised, and the results presented. In the end, we simulated this process and the results compared with the experimental data.

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**Stabilization of mine tailings using biological induced precipitation methods for wind erosion control****Authors:** Farideh Ehsasi<sup>1</sup> ; Leon van Paassen<sup>2</sup><sup>1</sup> *Student*<sup>2</sup> *Associate Professor***Corresponding Authors:** fehsasi@asu.edu, leon.vanpaassen@asu.edu

Wind erosion (dust) is a severe problem for mine tailings industry, as it poses environmental and safety concerns to public. Biological induced precipitation methods are found to be able to improve the resistance of soil for wind erosion. In this study microbiologically carbonate precipitation (MICP) based on urea hydrolysis was used to stabilize the surface of different tailings materials. An experimental study was performed on soil-filled pans that were prepared using loosely packed tailings material and treated using percolation of reactive solutions. Penetration testing and calcium carbonate content analysis were utilized to optimize the treatment strategy and assess the strength and durability of the cemented crusts. The results were compared with the alternative, already existing treatment strategies using magnesium chloride and xanthan gum. The MICP treated pans showed an increase in strength and durability with increasing concentration of the cementation solution and

number of treatments. MICP treated pans showed higher durability upon wetting and drying cycles compared to existing treatment strategies.

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Poster + / 233

## Statistical prediction of waterflooding performance by K-means clustering and empirical modeling

**Authors:** Qinzhuo Liao<sup>1</sup> ; Gang Lei<sup>1</sup> ; Xu Liu<sup>1</sup> ; Liang Xue<sup>2</sup> ; Shuyu Sun<sup>3</sup> ; Shirish Patil<sup>1</sup>

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Statistical prediction is often required in reservoir simulation to quantify production uncertainty or assess potential risks. Most existing uncertainty quantification procedures aim to decompose the input random field to independent random variables, and may suffer from the curse of dimensionality if the correlation scale is small compare to the domain size. In this work, we develop and test a new approach, K-means clustering assisted empirical modeling, for efficiently estimating waterflooding performance for multiple geological realizations. This method performs single-phase flow simulations in a large number of realizations, and uses K-means clustering to select only a few representatives, on which the two-phase flow simulations are implemented. The empirical models are then adopted to describe the relation between the single-phase solutions and the two-phase solutions using these representatives. Finally, the two-phase solutions in all realizations can be predicted using the empirical models readily. The method is applied to both 2D and 3D synthetic models and is shown to perform well in the P10, P50 and P90 of production rates, as well as the probability distributions as illustrated by cumulative density functions. It is able to capture the ensemble statistics of the MC results with a large number of realizations, and the computational cost is significantly reduced.

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## Steady-State Liquid Permeability Measurements in Ultra Tight Rock Samples

**Authors:** Hadi Bagherzadeh<sup>1</sup> ; Hossein Khorshidian<sup>1</sup> ; S. H. Hejazi<sup>1</sup>

<sup>1</sup> *University of Calgary*

**Corresponding Authors:** shhejazi@ucalgary.ca, hadi.bagherzadeh1@ucalgary.ca, hossein.khorshidian@ucalgary.ca

Matrix permeability is one of the most important characteristics of reservoir rocks yet its accurate measurement is often challenging for ultralow permeable shale and tight formations. Permeability of these reservoirs is in the range of micro-Darcy to nano-Darcy and depends on several factors including confining stress, pore pressure, pore fluid, and temperature. Hence, determination of permeability values in these rock samples is prone to errors where some inconsistencies exist in reported permeability values in the literature. In permeability measurements of tight and shale rock samples, transient methods are preferred over steady-state approach due to their time efficiency. Transient techniques, such as pulse decay permeameters, rely on using gases on measuring permeability requiring additional assumptions and parameters, hence, inaccuracies in the measurement arise especially when the flow path sizes are comparable with the mean free path of gas molecules. The use of steady-state methods, which provides an accurate and reliable estimation of rock permeabilities in conventional reservoir rocks, is limited for ultra-tight samples due to the long run-times. The presence of a small dead volume in the apparatus, comparable to the pore volume of tight samples, also contributes to uncertainties of measured permeability. However, unlike transient methods, liquids can be used as the flowing fluids in steady-state approaches with much confidence. Herein, we present the results of a custom-built liquid permeameter, based on the steady-state approach that can accurately measure permeabilities in the range of micro and nano Darcy. A core flooding apparatus is custom-built to nearly zero dead volumes and minimum upstream volume which consequently speeds up the steady-state measurements. Experiments are done with dodecane as the measuring fluid and different tight rock types including carbonate, sandstone as well as shale rock samples with permeabilities in the range of 10  $\mu\text{D}$  to 10 nD. The new permeameter generates repeatable permeability values with maximum error of 5%. The experimental run time is less than one week for samples with the permeability above 1  $\mu\text{D}$  and maximum three weeks when the permeability is below 1  $\mu\text{D}$ .

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MS14 / 637

## **Stochastic 3D microstructure modeling for three-phase electrode materials with an emphasis on transport relevant characteristics**

**Authors:** Matthias Neumann<sup>1</sup> ; Volker Schmidt<sup>1</sup>

<sup>1</sup> *Ulm University, Institute of Stochastics, D-89069 Ulm, Germany*

**Corresponding Authors:** volker.schmidt@uni-ulm.de, matthias.neumann@uni-ulm.de

We use parametric stochastic 3D microstructure modeling to generate digital twins representing the complex microstructure of three-phase electrode materials observed by tomographic imaging. For this purpose, we consider two models based on methods of stochastic geometry. The first model is based on random networks, while the second one is based on excursion sets of two independent Gaussian random fields [1]. Both models, for which we have derived new relationships between model parameters and morphological characteristics, are fitted to 3D image data representing anodes in solid oxide fuel cells consisting of nickel, a ceramic phase (Yttrium-stabilized zirconia) and pores. Model validation is performed with respect to the transport relevant microstructure characteristics mean geodesic tortuosity and constrictivity, *i.e.*, a geometrically defined radius of the characteristics bottleneck normalized by the median value of the continuous phase size distribution. Moreover, permeability of the pore space and effective conductivities of the solid phases are numerically simulated using Fourier methods [2]. This allows us to investigate quantitative relationships

between morphological characteristics and effective properties, which is an essential question in the field of heterogeneous materials [3], for the considered anode materials. Additionally, we show that excursion sets of two correlated Gaussian random fields can be used to model the microstructure of gas-diffusion electrodes consisting of silver, polytetrafluorethylen and pores [4]. We present a method for parameter estimation by means of two-point cross-coverage probability functions. After having fitted the model to 3D image data, model validation shows that mean geodesic tortuosity and the geometrically defined radius of the characteristic bottleneck are nicely reproduced.

**Time Block Preference:**

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**Poster + / 231**

## Stochastic homogenization of some porous media models

**Author:** Hakima Bessaih<sup>1</sup>

**Co-authors:** Razvan Florian Maris<sup>2</sup> ; Yalchin Efendiev<sup>3</sup>

<sup>1</sup> *University of Wyoming*

<sup>2</sup> *Alexandru Ioan Cuza University of Iasi*

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We will be dealing with various models from porous media stemming from applications in filtration processes. Our models includes the reaction diffusion and the convection diffusion models coupled with a stochastic differential equation.

Our models are highly heterogeneous in time and space.

Our main result consists of deriving the macroscale equation. We show that the resulting macroscale equation is deterministic. The convergence analysis involves the cell problem and the invariant measure of the stochastic differential equation.

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## Strain evolution, faulting, and slow slip in Draupne shales

**Author:** Aldritt Scaria Madathiparambil<sup>1</sup>

**Co-authors:** Fredrik Kristoffer Mürer<sup>2</sup>; Kim Robert Tekseth<sup>2</sup>; Nicolaine Agofack<sup>3</sup>; Pierre Cerasi<sup>4</sup>; Jessica McBeck<sup>5</sup>; Francois Renard<sup>5</sup>; Basab Chattopadhyay<sup>6</sup>; Dag Werner Breiby<sup>7</sup>

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New developments in carbon capture and storage (CCS) technology are under constant demand, and current initiatives focus on evaluating the possibility to store carbon dioxide (CO<sub>2</sub>) below the seabed in the North Sea 1. The Draupne Formation is a promising candidate and acts as a caprock for deeper reservoirs [2]. Injection of CO<sub>2</sub> in such formations could cause changes in the in-situ stresses, resulting in fault reactivation or the creation of microfractures, and thus alter the performance of the caprock. The ability of shale caprock seals to prevent CO<sub>2</sub> leakage is a major concern for the geological storage of anthropogenic CO<sub>2</sub> emissions, however, the micromechanisms of the crack formation are not well understood.

Time-lapse synchrotron-based micro computed tomography ( $\mu$ CT) imaging has made it possible to study non-destructively the mechanical behaviour of rocks. By using an advanced rock deformation apparatus, the HADES triaxial rig [3-5] (Fig. 1a), conditions similar to those found in the natural environments at kilometer depths below the seabed can be reproduced during dynamic  $\mu$ CT experiments.

Here, we combine  $\mu$ CT and digital volume correlation (DVC) analysis [4] to measure the mechanical properties of a Draupne shale sample when loaded under reservoir conditions. In the sample, brittle failure occurred and slip accumulated on the newly created fault [6]. Detailed quantitative analysis of the data using DVC reveals complex temporal three-dimensional (3D) patterns of the evolving strain. Interestingly, changes in the linear region of stress-strain are found to be irreversible. Intermittent bursts of deformations at apparently random locations are observed, and they gradually converge to a localized major fracture plane developing across the sample (Fig. 1c). Localization of the strains before the formation of the macroscopic fault can be quantified. Creep on the major fracture was observed which shows that slow deformation in shales can be related to the slip-on faults and not only to bulk creep. Visualizations and calculations of the volumetric and von Mises strains help quantifying the evolving strain within the sample (Fig. 1d).

Time-resolved  $\mu$ CT in combination with DVC reveals the local mechanics in Draupne shale, and is a promising method to understand the microstructural geomechanics of these rocks for the application of CO<sub>2</sub> sequestration.

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### Acknowledgments

The Norwegian Research Council is gratefully acknowledged for funding through Petromaks2 (90374300 “CuttingEdge”), FRINATEK (285182 “4D-CT”), and its Centre of Excellence funding scheme (262644 “PoreLab”).

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MS3 / 669

## Strength and stability of fractured rocks

**Author:** Srutarshi Pradhan<sup>1</sup>

<sup>1</sup> *Researcher, PoreLab, NTNU*

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Strength and stability of rocks are essential information for engineers and operators working in the field like petroleum production, geothermal installation and underground CO<sub>2</sub> storage. During operations, sometimes fractures open-up at the well-boundaries and fractures are mostly seen as “disturbing elements” for the stability of wells and well-operations. It is a real challenge to plan a drilling operation in fractured-reservoirs (like chalk reservoirs) due to the presence of natural fracture network -drilling must be done in a controlled manner so that the well-integrity is not disturbed. Therefore, we need a better understanding on how pre-existing fractures can reduce the strength/stability of rocks. In addition, we need to develop tools for monitoring the opening-up of new fractures and their development. Our lab experiments [2,3] explored the stress-induced fracturing behavior of reservoir rocks during fluid injection scenarios. Using the acoustic emission (AE) monitoring system, we could count new fractures (micro-cracks) and track the major fracture propagation. In addition, we have developed a discrete element model (DEM) simulation code based on Fiber bundle model [4,5] to analyze the role of fractures (damage) on the strength/stability of porous rocks. Our simulation code can take into account both long-range and short-range load-sharing scenarios [6,7].

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MS13 / 191

## Study of convective drying of a mortar with a paste cover by NMR and MRI

**Authors:** Hicham Dialla<sup>1</sup> ; Benjamin Maillet<sup>2</sup> ; Alban Gossard<sup>3</sup> ; Jean-Baptiste Champenois<sup>4</sup> ; Philippe Coussot<sup>2</sup>

<sup>1</sup> CEA, DES, ISEC, DMRC, Univ Montpellier, Marcoule, France - Lab. Navier, Ecole des Ponts, Univ Gustave Eiffel, CNRS

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The convective drying of a composite system made of a porous medium covered with a paste is a situation often encountered with soils, building, cultural heritage materials [1] and recently in decontamination of cementitious materials in nuclear facilities [2]. The aim of this study is to understand the convective drying behaviour of an initially saturated mortar. For simple porous systems (soils, bead packings, etc) the drying rate is constant during a long first period, thanks to capillary effects tending to redistribute homogeneously the liquid and thus continuously transport liquid towards the free surface of the sample where it evaporates. This is followed by a second period of drying rate decrease, generally associated with the development of a dry front [3]. For our mortar the drying rate continuously decreases from the beginning of the test, indicating a process in which the driving force is not capillarity. Yet, the spatial distribution of moisture content in mortar during drying obtained from Magnetic resonance imaging reflects a homogeneous desaturation of the sample, showing that there is a driving effect throughout the sample. At last, dynamic relaxometry by Nuclear Magnetic Resonance gives us the distribution of relaxation time in the system while it dries, which allows to know the history of pore emptying in time. The capillary pores (50-600 nm) appear to dry first, followed by inter-CSH pores (2-10 nm), while intra-CSH pores (0.5-1.8 nm) remains saturated. We suggest that the drying of such a material relies on the slow diffusion of the liquid through a continuous structure of inter-CSH pores. We also explored the drying behaviour of a mortar sample covered with an initially wet paste layer.

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MS5 / 781

# Study of the Combined Effect of Reservoir Souring and Scale Formation in hydrocarbon reservoirs

**Author:** Ali Mahmoodi<sup>1</sup>

**Co-authors:** Mohammad Reza Alizadeh<sup>1</sup> ; moein Jahanbani veshareh ; Hamid M. Nick<sup>2</sup>

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Seawater flooding, is a widely used improved oil recovery technique in oil reservoirs. Due to presence of sulfate (SO<sub>4</sub><sup>2-</sup>) in seawater, this technique can be associated with two side effects. The first side effect is the formation of various types of scale (e.g. BaSO<sub>4</sub>, CaSO<sub>4</sub>, and SrSO<sub>4</sub>) due to the incompatibility of seawater and formation brine that reduces permeability both in the reservoir and wellbore. For example, seawater containing SO<sub>4</sub><sup>2-</sup>, with field water rich in Ba<sup>2+</sup> may cause BaSO<sub>4</sub> scale precipitation both within the formation and also on co-production at the wellbore[A]. Second, the activity of sulfate reducing bacteria (SRB) may result in bio-conversion of sulfate into hydrogen sulfide, a hazardous[B] and corrosive gas. In case both of these processes are possible, they will compete for sulfate and one may limit the other. Therefore, it is important that the both are studied simultaneously. Furthermore, use of souring mitigation strategies can also affect the availability of sulfate through different pathways[C], which in turn calls for the necessity of a comprehensive simulation of all the processes. What makes this complex is that the microbial activity happens through one-way chemical reactions, which is the microorganisms consume sulfate among other things to generate the products, especially hydrogen sulfide in case of SRB. However, scaling happens through equilibrium processes, which mean the reaction path is determined based on the comparison of a state with the equilibrium state. Hence, the microbial reactions can heavily disturb possibly already existing equilibrium of sulfate with other ions and minerals in the reservoir.

In this work, we first present a model that simulates reservoir souring and mitigation together with scale formation simultaneously. Next, we use available experimental data in the literature to validate the model. A series of simulations are then conducted to identify the important parameters that control hydrogen sulfide production, scale formation, and the competition between them. The effect of scaling on porous media properties (porosity and permeability) is then discussed. Additionally, we discuss the possibility of optimizing souring mitigation strategies such that it doesn't trigger severe scaling.

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MS22 / 358

**Study of the impregnation process of electric engines' rotors with a reactive thermosetting resin: modeling and characterization of multi-physical coupling****Author:** Amélie Moisy<sup>1</sup>**Co-authors:** Sébastien Comas-Cardona<sup>1</sup>; Nicolas Désilles<sup>2</sup>; Pascal Genevée<sup>3</sup>; Jere Kolehmainen<sup>3</sup><sup>1</sup> *Research Institute in Civil Engineering and Mechanics (GeM), UMR CNRS 6183*<sup>2</sup> *Polymers, Biopolymers, Surfaces laboratory (PBS), Normandie Université, INSA Rouen Normandie, CNRS UMR 6270, 685*<sup>3</sup> *Renault***Corresponding Authors:** amelie.moisy@hotmail.fr, nicolas.desilles@insa-rouen.fr, jere.kolehmainen@renault.com, sebastien.comas-cardona@ec-nantes.fr, pascal.p.genevee@renault.com

As part of its development in the electric mobility market, the Renault Group assembles its own electric engines. The rotor is the mobile part of the electric rotating machine.

A rotor is mainly composed of a steel core wound by insulated copper wires. During the rotor production, the winding is impregnated with an acrylate-based thermosetting resin in order to:

- maintain the copper wires packed and avoid the relative movements due to electromagnetic, vibrational and centrifugal forces (rotation speed can rise up to 12000 rpm).
- improve the quality of the insulation,
- resist to chemical attacks and moisture,
- improve the thermal conductivity of the winding.

The impregnation process is complex, including an immersion of the winding into a liquid resin bath and controlled temperature settings to facilitate the flow and the polymerization. As opposite to many and well-known composite processes, the processing of the rotor does not involve a pressurization to facilitate the resin flow between the fibers (of few millimeters of diameter) and to avoid bubbles and unfilled areas in the winding. This suggests that capillary and gravity forces play a significant role into the rotor impregnation. The objective of the study is then to evaluate the impregnation quality of the windings within such processing conditions. It will require to characterize and to simulate a multi-materials and multi-physics process in which phenomena such as heat transfer, polymerization kinetics and resin flow are strongly coupled.

The defined research plan considers 2 submodels: heat transfer and flow. The first one includes the heat transfer taking into account the exothermy of the reaction and the second the mass conservation and resin flow, taking into account the chemo-rheology and the capillary effect 1.

Regarding the flow sub-model, the choice of a Darcy-type approach [2] or not is not obvious as the separation of scale is not that well defined (the number of wires is below 200).

In parallel, the material properties have to be characterized: polymerization kinetics, rheology evolution according to time and transformation [4] and capillary forces according to the geometry variations [5].

The developed simulation and characterization approaches will be presented, especially for the capillary impregnation aspect. Indeed, a capillary rise set-up has been developed to evaluate the impact of various parameters such as wire size, surface preparation or wires drying on the impregnation. Then material properties associated to capillary phenomena (contact angles and surface tension) has been evaluated to link experiments to analytical models [3].

**Time Block Preference:**Time Block B (14:00-17:00 CET) **References:**

1 Loïc Chevalier. Prise en compte des effets capillaires dans la modélisation par éléments finis et level-set de l'imprégnation dans les milieux fibreux. PhD thesis, Ecole des Mines de Saint Etienne, France, 2019.

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- [3] N. Fries and M. Dreyer. The transition from inertial to viscous flow in capillary rise. *Journal of Colloid and Interface Science*, 327(1):125–128, 2008.
- [4] M. Ivankovic, L. Incarnato, J. M. Kenny, and L. Nicolais. Curing kinetics and chemorheology of epoxy/anhydride system. *Journal of Applied Polymer Science*, 90(11):3012–3019, 2003.
- [5] Jean-marc Senecot. Etude de l'imprégnation capillaire de tissus de verre. PhD thesis, Université de Haute Alsace, France, 2002. **Acceptance of Terms and Conditions:**

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**Poster + / 691**

## Study of the mobility of zero-valent iron nanoparticles in porous media – Effect of grain size and composition

**Authors:** Nathaly Lopes Archilha<sup>1</sup> ; Raoul Djou Fopa<sup>2</sup> ; Tannaz Pak<sup>3</sup> ; Tiziana Tosco<sup>4</sup>

<sup>1</sup> *Brazilian Center for Research in Energy and Materials*

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<sup>3</sup> *Teesside University*

<sup>4</sup> *Politecnico di Torino*

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This work aims at advancing our understanding of the mobility and entrapment of nanoparticles (NPs) in porous media. The findings of this study are important for remediation of contaminated groundwater using nanoparticles (e.g. zero-valent iron). We focus on identifying the key NP transport mechanisms at pore scale in a non-destructive way using X-ray computed micro-tomography (X-ray micro-CT). In the modelling of particle transport in porous media, several key particle entrapment mechanisms are commonly considered, these are namely ripening, site blocking, straining, attachment, and detachment. These studies use data such as breakthrough curves, particle and grain size distribution as input to calculate the relevance and extent of the above-mentioned mechanisms<sup>1</sup>. In this work, the objective is to use X-ray micro-CT to directly observe the pore-scale mechanisms involved in particle mobility.

We report the outcomes of an experiment that was performed on small columns packed with grains of different size ranges and different compositions (fine sand, coarse sand, carbonate, and a mixed sample of carbonate and sand). The columns were initially saturated with water. A suspension of NP (zero-valent iron) was then injected in the columns, followed by a water flush step that removed the mobile particles. X-ray micro-CT imaging was performed at this stage. Our experimental dataset comprises 3D micro-CT images of these four columns.

The collected images have captured the distribution and characteristics of the trapped NP clusters. To analyse these images, we used the following workflow. The analysis started from filtering the collected images to remove the measurement noise. We then performed segmentation using a range of algorithms including watershed and WEKA segmentation. Subsequently, the segmented pore and NPs phases were quantitatively analysed. The image analysis was performed using Avizo and ImageJ software packages.

The focus of this work is developing a quantitative understanding of the effect of NP entrapment on the properties (e.g. porosity, permeability, and tortuosity) of porous media with different grain structures and compositions. We used the pore network modelling (PNM) module implemented in the Avizo software to extract PNMs from the 3D images of the segmented pore phase before and after the NP injection process.

For the samples under investigation the calculated properties (porosity, permeability, and tortuosity) agree with the range of values reported in the literature for similar pore systems. Our study shows that the permeability reduces by an order of magnitude because of this NP injection. Although the calculated tortuosity displays an increase, as expected, the extent of this increase is not significant (less than 10%). The number of pores shows a slight increase while a significant reduction in pore-throat count is observed. The latter can be associated with clogging of pore-throats because of NP injection.

This work uses the numerical micro- and nanoparticle transport, filtration, and clogging modelling suite (MNM's 2021) to simulate this 1D column experiment and to specifically study the mechanisms

involved in NP mobility at the pore scale. Based on model results, mechanical straining is suggested to be the key mechanism responsible for NP mobility in this study.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

1. Hosseini, S. M. & Tosco, T. Transport and retention of high concentrated nano-Fe/Cu particles through highly flow-rated packed sand column. *Water Res.* 47, 326–338 (2013).

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Poster + / 235

## Study on Oil Recovery Effect and Mechanism of the Supercritical CO<sub>2</sub> Huff-n-Puff Process in Tight Cores with Nuclear Magnetic Resonance (NMR)

**Authors:** Chaofan Li<sup>1</sup> ; Dongxing Du<sup>1</sup>

<sup>1</sup> *Qingdao University of Science and Technology*

**Corresponding Authors:** du-dongxing@163.com, 1049220228@qq.com

At present, we are facing two challenges of the increasing demand on energy resources and the increasing discharge of CO<sub>2</sub>. In one hand, the newly exploited oil and gas reserves consist of high proportion of low permeability reservoirs, which are difficult to be developed. On the other hand, astonishing amount of CO<sub>2</sub> is discharged into the atmosphere accompanying the fossil energy consumption in industrial activities, which results in the serious greenhouse effect. Due to the capability not only on enhancing oil recovery from unconventional oil reservoirs but also on storing large amount of greenhouse gas in underground formations, CO<sub>2</sub> huff-n-puff process is becoming an exciting research topic in recent years.

In this paper, two sandstone cores with 2.5cm in diameter, 7cm in length and gas permeabilities of 1.7mD and 2.6mD were employed and liquid paraffin was employed as the oil phase. After saturating the tight cores with the oil, CO<sub>2</sub> huff-n-puff processes were carried out in both cores to see the effect of soaking time on oil recovery rates under the conditions of 50°C and 25MPa. For core No.1, the soaking period is 1-day, while the soaking time was set to 5-day for core No.2. To understand the oil recovery mechanism of the Supercritical CO<sub>2</sub> (ScCO<sub>2</sub>) huff-n-puff process, both cores were cut half after the completion of the process and the oil distribution in the entire core as well as the front half (the part close to the CO<sub>2</sub> injection and discharge hole) and back half of the core were scrutinized with help of the Nuclear Magnetic Resonance (NMR) measurement.

Following conclusions have been obtained,

- 1) The oil recovery rate after 5 days is 17.2%, which is higher than 15.2% after 1 day's huff-n-puff process, indicating the longer soaking time could explore more oil from the tight cores at the first cycle of huff-n-puff process.
- 2) NMR measurement results show that more oil in the large pore space (pore-throat radius larger than 0.05μm) of the core is produced after the completion of ScCO<sub>2</sub> huff-n-puff process, while the oil phase in the space with smaller pore-throat sizes is rarely mobilized. The NMR results further show that the oil content in the large pores of the front part is obviously lower than that of the back part of the core, which indicates that a round of huff and puff operation mainly produced the oil in the large pore spaces from the front part of the core, while a considerable part of the oil in the rear core has not been effectively developed
- 3) Extended huff and puff time can significantly improve the oil recovery efficiency of the front part of the core, but there is little difference between the peak values of NMR test curves of 5-day and 1-day huff and puff process at the back part of the core, which indicates that extended huff and puff time has better oil production effect on the front part of the core.

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MS12 / 304

**Study on poromechanical problems of hydrate sediment during phase transition process****Authors:** Linlin Wang<sup>None</sup> ; Xiaoliang Dai<sup>None</sup> ; Shuitao Zhang<sup>None</sup>**Corresponding Authors:** 13298444096@163.com, daixiaoliangcup@163.com, linlin.wang@cup.edu.cn

This paper establishes a comprehensive model to describe the deformation of hydrate sediment involved in the hydrate recovery process. It combines two parts: phase transition of hydrate in porous media and unsaturated poromechanics. This model considers that the substances in the pores are modeled as two phases: the hydrate solid phase, and free gas stay in continuous liquid water as individual gas bubbles namely the equivalent fluid phase. Because of capillary effects between hydrate and fluid, the phase equilibrium conditions in fine sediments are shown as a zone rather a line in p-T diagram. When recovery hydrate by different stimulation methods, we calculate the deformation of hydrate sediment respectively by using this comprehensive model. In undrained condition, the pore pressure rises significantly during the hydrate dissociation process. This is because the gas released from the melting hydrate cannot be expelled from pores. This build-up of pore pressure lead to the deformation of the sediment, it also increases the hydrate dissociation temperature, and thus more heat supply is required when all the hydrates are dissociated. Finally, we compared the results of different recovery methods and got those conclusions: the thermal stimulation method in drained condition that leads to least deformation, and thus it's the favorable way. But in undrained condition, the thermal stimulation method results in the largest deformation and so it's the dangerous way in low permeability hydrate sediment.

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Poster + / 670

**Study on the Production Characteristics of Shale Oil using Machine Learning: Case Study of Jimsar Field****Author:** Wanhang Guo<sup>None</sup>**Co-author:** Jianchun Xu <sup>1</sup><sup>1</sup> *China University of Petroleum (East China)***Corresponding Authors:** 20170048@upc.edu.cn, guowh0808@163.com

The production rate for horizontal wells of shale oil is low. In order to achieve the economic and effective development, hydraulic fracturing technology is often adopted. After hydraulic fracturing, wells have a high production rate in the initial stage. After a period of production, the production rate

will drop rapidly, and then will maintain at a lower level for a long period of time. The study of decline characteristics of horizontal wells is significant. We collected the development data of 94 horizontal wells in Jimsar field. Some classical decline curves methods like “power law loss ratio” rate decline model, stretched exponential equation and Duong decline curve are all used to fitting the production history. The fracture-control decline rate is proposed to describe the initial stage decline degree. The machine learning method is used to explore the relationship between some important parameters (oil reservoir encountering rate, ratio of class-I formation, ratio of class-II formation, ratio of class-III formation, ratio of class-IV formation, reserve abundance, fracturing treatment parameters) and fracture-control decline rate. Support Vector Machine and BP neural network are used to predict 1 year cumulative oil. The result shows that the class-I formation (high permeability and porosity) and class-IV (low permeability and porosity) formation have the largest effect on the cumulative oil.

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MS12 / 165

## **Study on the coupling mathematical model of gas-water two-phase seepage and wellbore pipe flow in fractured horizontal Wells in volcanic gas reservoirs**

**Author:** Fu Cheng<sup>None</sup>

**Co-author:** Qingyuan Li <sup>1</sup>

<sup>1</sup> 13244696989

**Corresponding Author:** cheng\_fu111@163.com

The volcanic gas reservoir of Xushen gas field is the main production layer of natural gas development in Daqing reservoir in the future. Although this kind of gas reservoir is rich in resources, it is difficult to develop because of its poor physical property and complicated seepage mechanism. Most of the gas wells are fractured horizontal wells, with low single well production, small well control dynamic reserves, water layer generally developed at the bottom, and low stable production capacity of gas Wells. Therefore, it is of great significance to study the gas-water two-phase productivity of fractured horizontal Wells in volcanic gas reservoirs.

Based on the principle of gas-water two-phase seepage and the non-linear seepage mechanism of gas reservoir, according to the principle of equal flow rate and momentum theorem, combined with the nature of gas and the actual gas state equation, taking into account the internal friction pressure drop of wellbore, acceleration pressure drop and ball seat pressure drop, this paper establishes a matrix-natural fracture-artificial fracture-wellbore volcanic gas reservoir fractured horizontal well gas-water two-phase seepage and wellbore pipe flow coupling mathematical model, and solves the model by VB programming. The productivity and pressure distribution are predicted. At the same time, the influencing factors of gas-water two-phase productivity of fractured horizontal wells in volcanic gas reservoirs are studied. It is found that the degree of influence of stress sensitivity coefficients of different media on productivity is natural fracture or secondary fracture stress sensitivity coefficient, artificial main fracture stress sensitivity coefficient and matrix stress sensitivity coefficient from large to small. The high-speed nonlinear coefficient has great influence on the productivity, while the starting pressure gradient has little influence on the productivity. Finally, the accuracy of the model is verified by using the production data of five existing horizontal wells, with an average accuracy of 90.28%. The results show that the research results in this paper have certain reference significance for productivity prediction of fractured horizontal wells in low permeability volcanic gas reservoirs.



**Time Block Preference:**Time Block A (09:00-12:00 CET) **References:****Acceptance of Terms and Conditions:**Click here to agree **Newsletter:**I do not want to receive the InterPore newsletter **Student Poster Award:****Poster + / 537****Study on the reuse of shut-down offshore platform****Authors:** hongbo huo<sup>None</sup> ; Jinman Li<sup>None</sup> ; shiming he<sup>None</sup> ; zhong li<sup>None</sup> ; xiaocheng zhang<sup>None</sup>**Corresponding Authors:** lizhong@cnooc.com.cn, zhangxch3@cnooc.com.cn, hesming@sina.com, lijn17@cnooc.com.cn, huohb@cnooc.com.cn

In the next 20 years, there will be a large number of offshore oil fields to complete oil and gas exploitation. The removal of offshore platforms in resource exhausted areas is the mainstream treatment method at present. However, it is expensive to use large-scale offshore equipment, and there is little research on the reuse of offshore platforms. Based on the analysis of the current situation of the reuse of offshore engineering structure, the advantages and disadvantages of the existing methods are compared, and combined with the needs of offshore oil enterprises, the use of offshore platform for offshore logistics transfer station, offshore gas storage, offshore laboratory and other purposes is proposed, and the internal factors restricting the reuse of shutdown platform are analyzed, such as wellhead demolition and oil and gas channeling channel plugging; external factors, such as the law It also puts forward the corresponding solutions. Although there are many constraints and there is still a long way to go for practical application, the good economic benefits and application requirements make the reuse of discontinued offshore platforms have great application prospects. This paper studies and prospects the reuse direction of the future stop production platform, which provides a reference for further mining economic benefits.

**Time Block Preference:**Time Block C (18:00-21:00 CET) **References:****Acceptance of Terms and Conditions:**Click here to agree **Newsletter:****Student Poster Award:****MS5 / 110****Studying viral aggregation in porous media****Authors:** Dong Zhang<sup>1</sup> ; Valentina Prigiobbe<sup>1</sup><sup>1</sup> *Stevens Institute of Technology***Corresponding Authors:** vprigiob@stevens.edu, dzhang18@stevens.edu

Viruses are generally found as aggregates in the environment. The aggregation is a natural process which helps viruses to survive in soil and sediments and provides them resistance to disinfection, when they are suspended in water. Aggregation distinguishes between homogeneous and heterogeneous. In the former viruses agglomerate among themselves; whereas in the latter they nucleate around a foreign particle. The formation of viral aggregates may facilitate transport of viruses as well as cause clogging of porous media. Viral agglomeration depends on the type of virus, solution composition, and the presence of particulate. If there are several works where the process is investigated experimentally, there are few attempts to describe it mathematically.

Here, we present a study which combines laboratory experiments and modeling to describe the formation and the evolution of viral aggregates. In particular, bacteriophage MS2 were used and tested under the effects of porous medium geometry, pH, ionic strength, and temperature. A microfluidic system was built with channels of various geometry and sinusoidal pore-throat. A mathematical model of particle aggregation based on the population balance equation (PBE) of the number of viral particles coupled with extended DLVO theory was developed to determine the interactions among viruses and the evolution of the cluster size. Preliminary results show that, an early aggregation occurs which controls the later evolution of the cluster size. Given a type of virus, pH and pore-throat shape are the important factors controlling the aggregation process.

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MS9 / 545

## Sub-resolution feature size classification based on tunable X-ray dark-field imaging

**Author:** Benjamin Blykers<sup>1</sup>

**Co-authors:** Caori Alejandra Organista Castelblanco<sup>2</sup>; Matias Kagias; Matthieu Boone<sup>3</sup>; Tom Bultreys<sup>2</sup>; Marco Stampanoni; Veerle Cnudde<sup>2</sup>; Jan Aelterman

<sup>1</sup> *Department of Geology, Ghent University*

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Pore space properties such as pore shape, connectivity and pore size distribution are key to understanding pore-scale processes. X-ray computed (micro-) tomography ( $\mu$ CT) has become one of the dominant techniques to non-destructively investigate this pore space in three dimensions.

In conventional attenuation-based  $\mu$ CT, the rule of thumb is that the achievable resolution is about three orders of magnitude smaller than the sample size (Cnudde and Boone, 2013). For heterogeneous materials with pores from the nanometer scale up to the millimeter scale (e.g. mineral building materials), this makes it impossible to visualize the entire pore space without taking (multiple) smaller subsamples. This trade-off between image resolution and sample size also forces modelers to make assumptions and generalizations about the unresolved, sub-resolution pore space.

In the last fifteen years, X-ray dark-field tomography has been explored as a technique to overcome this trade-off between resolution and sample size. Dark-field imaging is based on small-angle X-ray scattering (as opposed to X-ray attenuation) and has been shown to be sensitive to sub-resolution density variations (Pfeiffer et al., 2009). Such variations are typically caused by structures of interest like sub-resolution pores, inclusions, micro-cracks and other heterogeneities. Dark-field imaging can be performed using Talbot-Lau grating interferometry, speckle-based imaging, or edge illumination. Although the published research on dark-field imaging is very promising, only limited use cases have been published on quantifying sub-resolution feature sizes (Lynch et al., 2011; Yashiro et al., 2010).

In this work, quantitative information on sub-resolution feature sizes in the nanometer regime has been extracted, based on this dark-field modality of X-ray tomography using Talbot-Lau grating interferometry. A validation experiment was performed at the TOMCAT beamline (Swiss Light Source, Paul Scherrer Institut, Switzerland) (Stampanoni et al., 2007). Alumina particles with either pore sizes of 50 nm or 150 nm were mixed together in a tube with a diameter of 1.5 mm and imaged using grating interferometry at five correlation lengths ranging from 45 nm to 800 nm to cover the pore size ranges. The image voxel size was  $1.62^3 \mu\text{m}^3$ . With conventional absorption  $\mu$ CT, it was

not possible to distinguish particles with different pore sizes due to their very similar density. However, the behavior of the particles' dark-field response over the range of correlation lengths allows to classify sub-resolution pore sizes. This suggests that dark-field imaging can be calibrated to quantify sub-resolution feature sizes inside porous materials, overcoming the resolution limitations of  $\mu$ CT.

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 Yashiro, W., Terui, Y., Kawabata, K., Momose, A., 2010. On the origin of visibility contrast in x-ray Talbot interferometry. *Opt. Express* 18, 16890. <https://doi.org/10.1364/oe.18.016890> **Acceptance of Terms and Conditions:**

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MS25 / 150

## Suction Cup System-Dependent Variable Boundary Condition: Transient Water Flow and Multi-Component Solute Transport

**Authors:** Iael Raij-Hoffman<sup>1</sup> ; Diederik Jacques<sup>2</sup> ; Naftali Lazarovitch<sup>3</sup>

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<sup>2</sup> *Institute for Environment, Health, and Safety, Belgian Nuclear Research Centre (SCKCEN)*

<sup>3</sup> *Wylar Department of Dryland Agriculture, French Associates Institute for Agriculture and Biotechnology of Drylands, Jacob Blaustein Institutes for Desert Research, Ben-Gurion University of the Negev, Sede Boqer Campus, Midreshet Ben-Gurion, Israel*

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Suction cups are widely used in agricultural and environmental research and monitoring under the hypothesis that the samples chemistry represents the soil pore water solute composition around the cup location. The objective of this study was to analyze the sampling procedures that lead to the most representative sample for soil aqueous phase composition when using a falling head suction cup. This was achieved by simulating simultaneously the hydraulic and geochemical response of the suction cup sampled soil solution and its immediate surroundings when evacuated by a system-dependent variable boundary condition. Different soils, water contents, vacuum applications and suction cup internal volumes, as well as variable hydraulic conductivities of the ceramic cup were evaluated and their effect on the sampling rate and sample chemical composition reported. Model results showed that potential extracted soil solution volume depends on a combination on internal suction cup volume and vacuum applied, independently from soil type or water content. A linear relationship was defined between the ratio of the extracted sample to suction cup volumes and the initial applied vacuum, for all simulations. pH values and general chemistry of the sampled solution were found to be more similar to those in the soil when a porous cup system is filled until hydraulic equilibrium is reached. Following this, a small volume suction cup system with a high initial applied vacuum, which allows for faster sample collection, could be optimal.

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## Surface Complexation Modeling on the Electrochemical Interactions of Low Salinity Waterflooding in Sandstone Reservoir

**Author:** Hongna Ding<sup>None</sup>

**Co-authors:** Xinjian Tan<sup>1</sup>; Yaling Xu<sup>1</sup>; Jihong Zhang<sup>1</sup>

<sup>1</sup> *Northeast Petroleum University*

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Low salinity waterflooding (LSW) attracts increasingly attentions in recent years. It has been proposed that the enhanced oil recovery by LSW (or low salinity response) is triggered by the electrochemical interactions (e.g., electrostatic interactions, multiple ion exchange, chemisorption, etc.) between brine, rock, and oil. This study used the methodology of surface complexation modeling to characterize those electrochemical interactions when LSW was applied in a sandstone reservoir, as well to investigate the influential factors (e.g., ionic chemistry, quartz and kaolinite contents, acid and base numbers of oil, etc.) of low salinity response. The modeling results indicated that the electrical repulsions of sandstone and oil surfaces contributed to the detachment of oil from sandstone surface and hence the low salinity response. The results also suggested that (1) the negativity of sandstone showed a complex change with the increase of NaCl concentration (0.001-10.0 mol/L) and its maximum value reached at 0.1 mol/L NaCl concentration, while the negativity of oil decreased with the increase of NaCl concentration, especially, the decrease became very pronounced below 0.1 mol/L NaCl concentration, which resulted in a salinity threshold for low salinity response; (2) Both the negativities of sandstone and oil were enhanced with the presence of SO<sub>4</sub><sup>2-</sup> ions in the salt solution but were compromised by Ca<sup>2+</sup> and Mg<sup>2+</sup> ions; (3) The negativities of sandstone and oil increased with the increase of pH, especially from pH=5 to pH=7; (4) The negativity of kaolinite was extremely small in high salinity water, however, it was moderately smaller than that of quartz in low salinity water, indicating that the kaolinite charge change played important roles in low salinity response; (5) The negativity of oil seems to be greatly influenced by the base number compared to the acid number. The findings of this study might theoretically guide the application of LSW in sandstone reservoir.

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## Surface-washing of contaminated porous substrates

**Authors:** Francesco Paolo Conto<sup>1</sup>; Merlin Etzold<sup>1</sup>

**Co-authors:** Stuart Dalziel<sup>1</sup>; Julien Landel<sup>2</sup>

<sup>1</sup> *University of Cambridge*

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We present surface-washing experiments modelling the decontamination of porous substrates. Firstly, we report a protocol to manufacture well-defined porous media by sintering glass ballotini (< 1 mm) to form free-standing homogeneous porous plates or incorporating a non-porous solid glass backing and/or surrounding: the resultant samples are mechanically stable cuboids. The ability to incorporate directly a solid glass backing provides a method of preventing any liquid leaks through their lower surface. These bespoke porous media are then integrated into an apparatus used in a previous work which studied surface-washing decontamination of impermeable surfaces (Landel et al. 2016).

Before the start of the experiment, a dyed fluid is introduced to the porous substrate to simulate the region of contamination. The surface-washing is simulated by a thin (~1 mm) film of water flowing from a reservoir through a gap over an inclined porous-glass surface. The resulting interaction between the cleansing film flow and the contaminating dye is then tracked using dye attenuation, enabling us to analyse the contaminant field in space and time.

A novel feature of these experiments is our use of bespoke porous media sintered from glass ballotini to form either free-standing homogeneous porous plates or composite structures where a porous matrix is sintered onto a solid glass backing with (optionally) solid glass surrounds.

We report results for a range of scenarios, assessing the role of initial conditions and cleaning strategies, demonstrating the possibility of the decontamination process leading to a redistribution of the contaminant within the porous medium.

#### **Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

Landel, J., Thomas, A., McEvoy, H., Dalziel, S.: Convective mass transfer from a submerged drop in a thin falling film. *J.Fluid Mech.* 789, 630–668 (2016) **Acceptance of Terms and Conditions:**

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MS7 / 29

## **Swelling beyond Flory**

**Authors:** Jacques Huyghe<sup>1</sup> ; Eanna Fennell<sup>1</sup> ; Philip Poillot<sup>2</sup>

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Super absorbents are swelling to thousands of percent of strain. Apart from the important industrial applications of these materials, the scientific understanding of electromechanical coupling in these ionized gels are paramount in the scrutiny of mechanotransduction of biological tissue. Regular finite deformation finite element codes fail to simulate these extremely large deformations [6]. A special purpose mixed hybrid finite element code demonstrates its ability to simulate swelling gels down to stiffnesses of 10 kPa, typical for super absorbents [6]. The constitutive modelling of these gels challenges researchers with strong non-linearities [3-5]. The traditional separation of free energy in an elastic, mixing and ionic part is contradicted by experiments 1. In order to address these issues, new avenues of constitutive modelling are explored [4]. The coupling between electrical and mechanical events may have far-reaching implications in the mechanotransduction phenomena in biological tissues [7]. Indeed, living cells are very well known to respond to electric potential changes and their sensitivity to mechanical load may very well be mediated by electromechanical couplings in the extracellular matrix.

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## Synchrotron Microtomography Investigation of Nanoparticle Entrapment and Mobility in Porous Media

**Authors:** Tannaz Pak<sup>1</sup> ; Daphne Silva Pino<sup>2</sup> ; Alexander Wood<sup>3</sup> ; Luiz Fernando de Lima Luz Junior<sup>4</sup> ; Tiziana Tosco<sup>5</sup> ; Nathaly Lopes Archilha<sup>6</sup>

<sup>1</sup> Teesside University

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Study of the mobility of nanoparticles in sand columns (or core flooding) at laboratory scale provides a good basis for understanding processes important in environmental engineering and hydrocarbon recovery from subsurface resources. Both of these applications can involve multi-phase fluid flow in subsurface porous systems. In hydrology, column experiments are used, among others, to support the design of in-situ groundwater remediation processes including those involving mostly reactive nanoparticles. In oil industry, core flooding experiments are used to study enhanced oil recovery processes including the use of mostly non-reactive nanoparticles. Both these applications deal with large-scale processes; however, the fluid flow actually happens at pore-scale (mostly micro-meter scale). This makes small scale laboratory experiments of special importance.

Conventional column experiments use information such as the concentration of the species of interest (in this case, particles) at column inlet and outlet, pressure, etc. to indirectly infer the pore-scale processes that occur in a sample during a flow and/or particle transport experiment. X-ray computed micro-tomography (X-ray micro-CT) allows a greater degree of understanding with regards to pore-scale dynamics through a process of 4D imaging (3D images resolved in time).

This study aims to investigate the mobility and entrapment of zero-valent iron nanoparticles (nZVI) in porous media. Two types of sand-packed columns with different grain size distributions (coarse and fine) were studied. The experiments started by saturating the column with water and a subsequent injection of the nanoparticle suspension. A post water flushing was done to remove the mobile nanoparticles. Using an X-ray transparent flow cell allowed capturing a sequence of 3D images during the experiments. In our previous studies only one field of view was imaged at every

injection step (1, 2). A distinctive aspect of this experiment is that we decided to image the column in three segments by moving the micro-CT stage in Z direction. The three segments are then stitched together in the post-processing step. This gives us the chance to investigate the nanoparticle mobility profile along the entire column length at each time step, without compromising on the image resolution.

The collected images are filtered, segmented, and analysed to show the degree of nanoparticle mobility in these different samples, and to allow calculation of flow properties (e.g. permeability) based on the images collected before and after the nanoparticle injections. The existence of both mobile and non-mobile nanoparticle clusters was imaged in this experiment. At pore-scale, the trapped nanoparticles are mainly observed to occupy the pore-throats, i.e. the narrowest parts of the flow pathways. The injected nanoparticle suspension phase is not miscible with the water phase (initially occupying the pore-space) at first contact. Our images show the formation of a water film covering the sand grains in presence of the nanoparticle suspension phase, making water the wetting phase. The results of this experiment shed light on the pore-scale mechanisms involved in nZVI entrapment in porous media. Comparison of our findings for the coarse and fine sand samples will assist in improving the efficiency of nanotechnology-based groundwater remediation processes.

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## Targeted delivery of fertilizer in coarse textured soils using foam as carrier

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Agrochemicals and fertilizers are central to modern agriculture and are credited with the large increase of crop yield as part of the Green Revolution of the 1960's. Timely and targeted fertilizer application is an important component for reducing costs and minimizing unintended release to the environment and water resource pollution. The efficiency of highly mobile fertilizers (i.e., nitrate) is affected by drainage and preferential flow pathways that bypass root bearing soil volumes. We report a novel liquid fertilizer delivery method using foam as carrier. The highly controlled transport of foam (defined as a dispersion of gas in a continuous liquid phase) in coarse soils (most susceptible to unstable flows) offers a means for targeted delivery to desired root zone volumes at concentrations and flow geometry that minimizes losses and promote its uptake. As proof of concept we conducted transport experiments in cylindrical soil columns using foam and conventional fertilizer application. Our results show that foam-assisted fertilizer application decreased the leaching of fertilizer and improved its retention in the soil column potentially offering a vehicle for fertilizer delivery in soil.

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## **The Alento hydrological observatory: An advanced open-air laboratory to evaluate the impact of anthropogenic disturbances on ecosystem services in a Mediterranean catchment.**

**Authors:** Nunzio Romano<sup>1</sup> ; Carolina Allocca<sup>1</sup> ; Luisa Stellato<sup>2</sup> ; Sarah Schönbrodt-Stitt<sup>3</sup> ; Heye Bogena<sup>4</sup> ; Paolo Nasta<sup>1</sup>

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Across the Mediterranean region, there is a need to obtain an in-depth understanding of the impacts of climate seasonality (drought) and land-use (including wildfires) on ecosystem services related to the hydrological cycle (contaminant transport, soil erosion, etc.), especially in hilly-mountainous catchments that can be more sensitive to imbalances in the management of land and water resources. A valid contribution to the development of sustainable management strategies and the prediction of the future condition is the integration of ground-, proximal-, and remote sensing-based monitoring activities together with diverse scientific expertise in the "Alento" hydrological observatory (southern Italy). This observatory was established in 2016 to provide large soil and hydrological datasets for Mediterranean environments and comprises two study sites (MFC2, agricultural use on clay soil; GOR1, forested site on loamy andic soil) instrumented with soil sensor networks (SoilNet) and cosmic-ray neutron probes (CRNP). Hundreds of disturbed and undisturbed soil samples were collected along transects in the catchment and also in the test sites at the nodes of regular 25-m×25-m grids to determine soil physical and hydraulic properties in these test sites. Here we will present the most recent investigations underway in the Alento observatory.

Data retrieved from the ground-based sensing systems are being integrated with dual polarimetric Sentinel-1 Synthetic Aperture Radar (SAR) data to provide effective identification of field-scale soil hydrological responses of sites with different characteristics. These activities have been firstly devoted to the development of a simplified calibration procedure of SAR-based parameters using local terrain attributes and sparse surficial soil moisture values. The developed site-specific calibration-dependent model was tested in MFC2 only for a short period in November 2018. Preliminary results show that the combined SAR + terrain model ( $R^2$  89%, RMSE 2.49 vol%) slightly outperforms the SAR-based model ( $R^2$  86%, RMSE 2.23 vol%) in terms of accuracy and agreement between observed and estimated values of near-surface soil moisture. Ongoing activities in MFC2 focus on the inverse



modeling in Hydrus-1D to simulate two supporting variables to calibrate SAR-based parameters: (i) sparse soil moisture data measured at the soil depths of 15 cm and 30 cm over the SoilNet locations, and (ii) downscaled field-scale soil moisture monitored with the CRNP. This task aims primarily at highlighting the effectiveness of integrating SAR-based measurements, topographic attributes, and CRNP data for mapping the near-surface soil moisture at a small scale with the advantage of being non-invasive and easy to maintain. Space-borne information on biophysical properties (i.e., vegetation) adds to the current efforts to enlarge the dataset. In both MFC2 and GOR1, systematic campaigns are carried out to measure the water isotope compositions of rain, soil, plant, shallow aquifer, and streamflow. This dataset helps verify the hypothesis of ecohydrological separation whereby distinct soil water pools supply either plant transpiration or groundwater recharge and surface runoff. Finally, this bulk of integrated sets of soil and hydrological data will serve as input into one- or three-dimensional hydrological models to investigate the interactions and feedback in the soil-vegetation-atmosphere continuum and obtain reliable scenario-based projections.

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## The Chemical/Biological Remediation of Non-Aqueous Phase Liquids in Heterogeneous Porous Microfluidic Devices

**Author:** Yan Li<sup>1</sup>**Co-authors:** Xu Wang ; Hangyu Li ; Jianchun Xu ; Shuyang Liu ; Xiaopu Wang<sup>1</sup> *Shandong Key Laboratory of Oilfield Chemistry, China University of Petroleum (East China), Qingdao 266580***Corresponding Authors:** shuyang\_liu@126.com, 20170048@upc.edu.cn, wxp@upc.edu.cn, wangxu314159@163.com, lihangyu@upc.edu.cn, yaneyli@outlook.com

Over the years, crude oil spills have occurred frequently, resulting in large amounts of toxic organic contaminants seeping down into the onshore soil-groundwater system. These non-aqueous phase liquids (NAPLs) can easily attach to soil particle surfaces and are difficult to eliminate, harming the environment continuously. Besides, the heterogeneity of soil makes the distribution of NAPL contaminants more complex, and it is difficult for conventional restoration agents to make sufficient contact with the NAPL in the low permeable zone, resulting in poor remediation. Therefore, proposing efficient and eco-friendly remediation methods of NAPL contaminated layers in heterogeneous soil-groundwater system is increasingly urgent.

In this study, a new eco-friendly chemical reagent and chemotactic bacteria were adopted to try to solve the problem above. The chemical reagent is dihydrolevoglucosenone, commercially known as Cyrene. Cyrene is a highlighted renewable and highly biodegradable cellulose-derived solvent, an attractive substitute to widely used toxic dipolar aprotic solvents. When added to water, Cyrene behaves as a hydrotrope, increasing the aqueous solubility of hydrophobic solutes to a great extent. Chemotactic bacteria have perceptions of contaminant concentration gradients in water and can make response to it by preferentially swimming towards regions of higher contaminant concentration. We designed a series of microfluidic devices with dual-permeability to simulate the heterogeneous soil contaminated with NAPL, and studied the efficiency of Cyrene (compared with the conventional surfactant Tween 80) and chemotactic bacteria to clear the NAPL contamination under different groundwater flow rates.

Our experimental results showed that though distilled water could displace a portion of the oil in the high permeable region of the microfluidic device, no explicit decrease of oil in the low permeable region was observed under different water flow rates. Better displacement effects were obtained in surfactant flooding. We found that the surfactant flooding with Tween 80 could produce fingering phenomenon in the low permeable area, and the fingering extent was related to water velocity and surfactant concentration. The flooding with Cyrene showed a better remediation effect compared

with water and Tween 80 at the same flow rate, and the higher the concentration of Cyrene, the less the NAPL residuals were in the chip. We also injected chemotactic bacteria suspension into the chip after the three types of fluids displacement above, and found that considerable bacteria tended to accumulate at the interface between the high and low permeable regions after water flooding; and more chemotactic bacteria were found in the low permeable region after the surfactant and Cyrene flooding. Our findings provide a novel idea to use chemotactic bacteria and green chemicals to improve the remediation of NAPL contamination in heterogeneous soil structures.

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## **The Effect of Surface Chemistry on Phase Behavior in Nanoporous Confinement: An Experimental Study of iso-Butane Isotherms**

**Authors:** Rami Alloush<sup>1</sup> ; Keerti Sharma<sup>1</sup> ; Mohammad Piri<sup>1</sup>

<sup>1</sup> *University of Wyoming*

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Understanding fluid phase behavior is of primary importance in different industries, including oil and gas exploration and production. It is known that nanoporous confinement plays a vital role in determining the phase behavior of fluids hosted in the rock pore space. While some quantitative understanding is available describing pure fluids' behavior in nanopores, surface chemistry's effects on fluids' behavior in confinement are not fully understood. In this work, the effects of adsorbent surface chemistry on nanoporous confinement were investigated using silica-based MCM-41 adsorbents with different degrees of surface modification. The isotherms of iso-Butane were generated using a novel gravimetric apparatus with four different MCM-41 adsorbents. Three of the adsorbents possessed varying degrees of surface modification with C1, C8, and C18 alkyl groups. The results of the adsorption tests in these three modified nanoporous materials are compared to isotherms measured with pure, unmodified, MCM-41 adsorbent with matching pore sizes. The isotherms were generated at temperatures 2, 8, 16, and 24 °C. The iso-Butane isotherms are also compared with the previously published n-Butane counterparts obtained with similar adsorbents. The results show that each adsorbent-adsorbate pair exhibit qualitatively different adsorption behavior due to varying interaction potentials between the adsorbent and the adsorbate. Moreover, this study demonstrates that the adsorption process is influenced by the molecular structures of the adsorbent and the adsorbate, particularly when capillary condensation is involved.

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## The Effect of Surface roughness on the Equilibrium Contact Angle in a Mixed-Wet Medium

**Authors:** Shahab Ghasemi<sup>1</sup> ; Mohammad Reza Rasaei<sup>1</sup> ; Sahar Bakhshian<sup>2</sup>

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Surface characteristics are important at the micro- and nano-scale level. Surface roughness is one of the main factors influencing the contact angle, as it increases the solid-fluid interfacial area and leads to the droplet impingement on sharp edges of a rough surface. In addition to the surface roughness, anisotropic wetting of chemically heterogeneous surfaces can be a driver to control the contact angle and hence the wetting behavior of a solid surface. In this study, the free energy lattice Boltzmann simulation is applied to investigate the effect of surface roughness and wettability heterogeneity on the equilibrium contact angle in pillar-like pattern surfaces. The rough surfaces are modeled with different pillar shapes and wettability ranging from hydrophilic to neutral wetting conditions. It is found that rectangular pillars lead to the contact line pinning, whereas frustum shapes facilitate the droplet movement.

Furthermore, the effect of relative surface roughness, roughness distribution, and the gravitational force on the equilibrium contact angle was studied. The length scale of the surface patterns is close to the droplet size, for which the Cassie-Baxter and Wenzel equations are not applicable. According to the results, the ratio of the roughness magnitude to the surface area of the droplet is a key factor influencing the equilibrium contact angle. Moreover, droplets on rough surfaces do not necessarily form with the absolute minimum energy. Since a droplet tends to pin on the edge of a pillar, a super-hydrophilic surface behaves as a hydrophobic one.

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## The Impact of Microscale Surface Roughness on Fluid Displacement Mechanisms and Residual Saturations in Porous Media

**Author:** Rumbidzai Nhunduru<sup>1</sup>

**Co-authors:** Amir Jahanbakhsh<sup>1</sup> ; Krystian Wlodarczyk<sup>1</sup> ; Omid Shahrokhi<sup>1</sup> ; Susana Garcia<sup>1</sup> ; Mercedes Maroto-Valer<sup>1</sup>

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Understanding the factors and mechanisms behind the trapping and immobilisation of residual saturations of carbon dioxide (CO<sub>2</sub>) and oil phases in the pore spaces of reservoir rocks during immiscible fluid displacement is vital for geological CO<sub>2</sub> storage and enhanced oil recovery (EOR) (1). The extent of trapping that occurs determines the success and efficiency of such subsurface operations. Whilst the objective of CO<sub>2</sub> storage operations is to maximise residual trapping of CO<sub>2</sub>, in EOR operations the objective is to suppress and minimise trapping of the oil phase (2). Fluid displacement processes and residual trapping are strongly influenced by the topological roughness of the porous rock (3). Currently, there is very limited data on the effects of surface roughness on fluid displacement processes (4). Accordingly, in this study we aim to quantify the effects of microscale surface roughness

on pore-scale fluid displacement processes.

To investigate the impact of surface roughness on pore-scale fluid displacement, immiscible displacement of air by water was conducted in a transparent glass micromodel at a flowrate of 8.33 $\mu$ L/min. The experiment was repeated three times to ensure reliability of results. The micromodel was fabricated using an ultrafast picosecond laser(5) and its pore network structure was comprised of cylindrical pillars 400  $\mu$ m in diameter arranged in a rhombohedral type of packing. Due to the inherent nature of the laser fabrication process, the walls and surfaces of the laser machined porous structure were rough textured. The average hillock height to pore depth ratio ( $\Omega$ ) for this micromodel was determined to be 5 $\mu$ m/50 $\mu$ m (10%) and the average measured surface roughness ( $S_a$ ) of the micromodel was 1.2 $\mu$ m. To isolate the effects of surface roughness on immiscible two-phase fluid displacement, a Direct Numerical Simulation (DNS) of the water-air fluid displacement process was performed for the same porous structure assuming completely smooth surfaces in OpenFoam using the Volume of Fluid (VOF) method.

Comparing the experiments with the numerical simulation, our results demonstrate that microscale surface roughness has a strong and significant influence on pore-scale fluid displacement mechanisms and its contribution should not be ignored. We show that at a hillock height to pore depth ratio ( $\Omega$ ) of 10%, surface roughness can increase residual saturations in such a porous structure by up to 49% from 4% in the numerical simulation to 53% in the micromodel with rough surfaces. This implies that surface roughness can promote the isolation and trapping of clusters of CO<sub>2</sub> in CO<sub>2</sub> storage operations, thereby increasing efficiency of the process. In EOR operations, the effects of surface roughness are detrimental as the sweep efficiency of displacement process is significantly reduced.

#### Acknowledgements

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## The Importance of Microstructure in Redox Flow Batteries

**Authors:** Mohammadjavad Shokriafr<sup>1</sup> ; Vahid,J Niasar<sup>None</sup>

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Producing energy from intermittent renewable energy sources has been developed over the past decades. One of the goals at the grid-scale is to provide sustainable energy output to the end-users. To this end, efforts must be done to store a huge amount of energy in robust batteries to provide stable and flexible electricity to the customers during peak hours. Redox flow batteries (RFBs) have been attracted attention to be one of the best candidates amongst electrochemical technologies [2]. RFBs are a highly efficient energy storage technology that uses reduced/oxidized states of species for charge/discharge purposes. The performance of RFBs is evaluated using a polarization curve which describes the relationship between the cell voltage and the current density [3]. At higher current densities, the cell voltage drops drastically as a result of mass transport loss, meaning that the mass transport controls the performance and power range of RFBs [4]. The poor design of electrode microstructure is one of the main causes of this occurrence. Hypothetically, it can be overcome by tailoring or engineering the microstructure of the electrode. Therefore, the reactive transport of ionic solution in RFBs has been simulated in pore-scale using Pore Network Modelling (PNM) to investigate the effect of the electrode microstructure on the performance of RFBs. This work focused on Hydrobromic Acid (HBr) RFBs that hydrogen gas is oxidized in the anode and the produced protons are transferred to the cathode to reduce bromine in the cathode. By use of two unstructured and structured pore networks and two interdigitated and flow-through flow patterns, the performance of RFBs were investigated. This work aims to optimize the electrode microstructure to broaden the power output of RFBs. Initial results show that species are mostly consumed in the outlet and the proximity of the membrane, mainly as a result of lower advective force in these areas. Consequently, bigger overpotentials were observed in these regions due to the lack of species supply. Also, concentration distribution in the flow-through pattern was more uniform than the interdigitated one. This can be explained by the electrolyte flow direction in the electrode and greater advection force in the flow-through pattern.

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**Poster + / 273**

## The Influence of Motility on Bacterial Accumulation in a Microporous Channel

**Authors:** Christoph Lohrmann<sup>1</sup> ; Miru Lee<sup>2</sup> ; Christian Holm<sup>3</sup>

<sup>1</sup> *University of Stuttgart*

<sup>2</sup> *University of Göttingen*

<sup>3</sup> *University of Stuttgart, Institut für Computerphysik*

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Swimming microorganisms are often encountered in confined, porous geometries where also an external flow is present, e.g. in filters or inside the human body. To investigate the interplay between

microswimmer motility, confinement and external flows, we developed a model for swimming bacteria based on point coupling to an underlying lattice Boltzmann fluid. With this implementation, straight swimming motion interrupted by random reorientation events reproduces the motility pattern of the run-and-tumble bacterium *E. coli*.

We present the application of the model to the study of bacterial dynamics in a simplified porous geometry: A rectangular channel with a single cylindrical obstacle. In accordance with experimental measurements, the results show asymmetric accumulation behind the obstacle only when the bacteria are active and an external flow is present<sup>1</sup>. We quantitatively compare bacterial densities from simulations to the experiments and investigate the physical mechanisms that lead to accumulation.

<sup>1</sup> M. Lee *et al.*: The Influence of Motility on Bacterial Accumulation in a Microporous Channel, *Soft Matter* advance article, 2021, DOI: 10.1039/D0SM01595D

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

M. Lee et al.: The Influence of Motility on Bacterial Accumulation in a Microporous Channel, *Soft Matter* advance article, 2021, DOI: 10.1039/D0SM01595D **Acceptance of Terms and Conditions:**

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MS13 / 411

## The Interplay of Spreading, Imbibition and Evaporation of Water Droplets on Nanoporous Surfaces

**Author:** Laura Gallardo<sup>1</sup>

**Co-authors:** Hugo Bellezza<sup>2</sup>; Juan Sanchez<sup>3</sup>; Patrick Huber<sup>4</sup>; Olivier Vincent<sup>5</sup>

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The study of fluid dynamics in nanoporous materials is nowadays a topic of great interest due to the often significantly modified thermal equilibrium and non-equilibrium properties of extremely spatially confined liquids compared to their bulk counterparts. However, fluid transport in nanoscale geometries plays also an increasing role in functional materials consisting of fluid-infused solids, such as supercapacitors and porous materials with integrated actuation, sensation and adaptive lubrication [2].

Here we present a study on the spreading of water droplets on nanoporous silicon as a function of time. The evolution of the droplet volume is analyzed theoretically and experimentally considering the evaporation and the radial imbibition of the liquid into the porous substrate. The scaling behavior of these quantities are qualitatively in agreement with phenomenological descriptions [3,4], however also substantial deviations compared to Molecular Dynamics simulations on this phenomenology are revealed [5]. Our experiments shall serve as a base for future studies employing electrowetting to control the competition of spreading and imbibition [6].

**Time Block Preference:**

**Time Block A (09:00-12:00 CET) References:**

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**Student Poster Award:****Invited & Keynote Speakers / 821****The Theory of Porous Media in Modelling Biological Tissues**

**Author:** Oliver Röhrle<sup>None</sup>

**Corresponding Author:** roehrle@simtech.uni-stuttgart.de

Experience and training are key aspects in medical practice. However, unlike other professions, medical practitioners have limited opportunities to perfect their skills before they must operate on people. Simulations help overcome such obstacles by carrying out virtual experiments, which would otherwise not be feasible. However, the human body is the most complex system known to mankind. The models for the simulations tend to be equally complex and computationally expensive. As humans are essentially a fluid saturated solid, empowering porous media models provides a useful and cost-effective tool for testing, analysing, planning and training of particular medical procedures. Simulating the vertebroplasty procedure, where a viscous fluid bone-cement is injected to the porous inside of vertebral bones to regain stability after the bone-cement has hardened, is one example. The key to use such simulations as a training / predictive tool is to validate the spread, i.e., the frontiers or the interfaces, of the injected bone cement (which is a PMMA), as it is injected, as well as the phase transition, i.e., the hardening process of the bone cement. Perfusion, i.e. flow of blood through capillaries into the heart or the organs, can be modelled using porous media as well. By including the transport equations, one can also model exchange processes occurring via advection, diffusion, and osmosis. Examples include vital processes like delivery of drugs to target organs, filtration of blood in the kidneys, gas exchange in the lungs, ion diffusion through the intervertebral disc, clotting of blood via thrombosis, etc., to name only a few. Especially linking the micro-scale chemical kinetics to tissue/organ scale porous media modelling is a powerful method for analysing, investigating and predicting (mechanical) behaviour of biological processes. There is a vast scope of applicability for porous media in the medical field, yet it is still largely untapped. Nevertheless, it has the potential to be one of the areas of mainstream research in the field, owing to its efficiency and versatility. In this talk, selected applications like the vertebroplasty and blood perfusion will be addressed.

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## The effect of the diffusion transport on CO<sub>2</sub>-water-rock reactions in CO<sub>2</sub> sequestration condition

**Authors:** Mingkun Chen<sup>1</sup> ; Yi Zhang<sup>1</sup> ; Yongchen Song<sup>1</sup>

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Due to the high storage capacity and the long-term sequestration safety, geological CO<sub>2</sub> mineralization in mafic and ultramafic reservoir has been widely researching via laboratory and field studies. Previous researches mainly focus on the dynamics of CO<sub>2</sub>-water-rock interactions in well-mixed constant pressure system, few studies have been carried out with pressure decay while CO<sub>2</sub> mineralization happened.

In this study, a series of high-temperature, high-pressure static experiments was conducted to simulate CO<sub>2</sub>-water-saturated olivine diffusion and reaction coupled processes investigating the impact of transport limitation, mineralization and grain size distribution. Once the injection of CO<sub>2</sub> in the formation, CO<sub>2</sub> diffuse into the brine, followed by the reaction with rock. During the long-term reaction, the CO<sub>2</sub> pressure continue to decrease monotonically, particularly showing a proposed linear relationship with time in the later time, and indicating that CO<sub>2</sub> is constantly consumed and permanently sealed. A one-dimensional diffusive mass transfer model has been used to attain the dynamic diffusion coefficients, quantifying the effect of mineralization and grain size distribution on the mass transfer of CO<sub>2</sub>, which are little higher than the pure diffusivities without reaction. And the comparison of Raman test results before and after the reaction at different heights show the dissolution of forsterite and chlorite, precipitation of magnesite, even in the deepest. The distribution and quantity of carbonate minerals along the depth direction, showing a non-uniform distribution trend resulting from localized and chemical gradient, was determined using XRD and total carbon analysis.

In combination, the results refine the understanding of coupled reactive and transport effects in geologic carbon sequestration, which is the primary mechanism in CO<sub>2</sub> mineral trapping process.

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Poster + / 272

## The effect of tomographic imaging resolution on residual saturations during the drainage process

**Authors:** Barzan Karimi<sup>1</sup> ; Mohammadreza Moshtari<sup>1</sup> ; Saeid Sadeghnejad<sup>1</sup> ; Frieder Enzmann<sup>2</sup> ; Michael Kersten<sup>2</sup>

<sup>1</sup> *Department of Petroleum Engineering, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*

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Nowadays, digital rock physics (DRP) has enabled us to obtain comprehensive and accurate information from porous media and a better understanding of physics at the pore scale. Advances in the micro-computed tomography technology ( $\mu$ CT) have led to high-quality, high-resolution images from rock samples. However, this increase in image quality or resolution raises imaging expenditures. Thus, the choice of a proper resolution during X-ray tomography is a challenging task and is



based on a compromise between accuracy and cost (money and time) [1,2]. It was shown that image resolution changes influence the permeability estimation from porous media [3,4]. Moreover, there is a critical resolution and sample size (or field of view, FOV) for accurate enough predictions of rock properties (e.g., porosity and permeability) when using DRP [5]. The representative elementary volume (REV) decreases and approaches a stable value at a very high resolution with improved image resolution [6]. Therefore, it is essential to obtain this critical resolution to determine the prediction accuracy.

This study investigates the resolution effect on the amount of residual saturation during brine/oil drainage in two sandstone and carbonate rock samples. Initially, high-resolution images of both rock samples are considered as the base  $\mu$ CT images. Several images at various resolutions are reconstructed by numerically changing the digital resolutions of the  $\mu$ CT images by ImageJ. The maximum sphere inscription algorithm extracts the pore network model (PNM) of each image. The amount of residual saturation is then calculated from the extracted PNMs by simulating the drainage process in OpenPNM and is then compared with that of high-resolution images.

Repeating the above steps for rock images with various resolutions shows that residual saturation gets stable above a resolution. This is because the large-size pores of the samples might not show to be in contact with other smaller pores at lower image resolutions. With increasing the resolution, the role of smaller pores and their connectivity to the pore network becomes more prominent. The results indicate that once the scan resolution is higher than a resolution for a given rock sample, the predicted residual saturations are accurate and representative. Thus, instead of acquiring high-resolution, high-quality  $\mu$ CT images at significant expenses, the results of residual saturation with relatively acceptable accuracy can be obtained at lower costs by finding the critical image resolution.

#### Acknowledgments

The third author (Saeid Sadeghnejad) gratefully acknowledges support from the Alexander von Humboldt Foundation for his visiting research at the Johannes Gutenberg University at Mainz (JGU), Germany.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

- 1 Leu, L., Berg, S., Enzmann, F., Armstrong, R. T., & Kersten, M. (2014). Fast X-ray micro-tomography of multiphase flow in Berea sandstone: A sensitivity study on image processing. *Transport in Porous Media*, 105(2), 451-469.
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MS24 / 30

## The effective boundary condition on a porous wall

**Authors:** Eduard Marusic-Paloka<sup>1</sup> ; Igor Pazanin<sup>1</sup>

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We derive the new effective boundary condition for the fluid flow in domain with porous boundary. Starting from the Newtonian fluid flow through a domain with an array of small holes on the boundary, using the homogenization and the boundary layers, we find an effective law in the form of generalized Darcy law. If the pores geometry is isotropic, then the condition splits in Beavers-Joseph type condition for the tangential flow and the standard Darcy condition for the normal flow. The result is rigorously justified by an appropriate error estimate.

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**Poster + / 686**

## The evolution of preferential flow paths during Enzymatically Induced Calcite Precipitation and its effect on the permeability

**Author:** Felix Weinhardt<sup>None</sup>

**Co-authors:** Jingxuan Deng<sup>1</sup>; Nikolaos Karadimitriou<sup>2</sup>; Johannes Hommel<sup>1</sup>; Robin Gerlach<sup>3</sup>; Holger Class<sup>1</sup>; Holger Steeb<sup>4</sup>

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Enzymatically Induced Calcite Precipitation (EICP) in porous media can be used as an engineering option to achieve targeted precipitation in the pore space. It is associated with an alteration of porosity and, consequently, permeability. A major source of uncertainty in modelling EICP is in the quantitative description of permeability alteration due to precipitation, based on commonly applied porosity-permeability relations 1. To improve these relations for REV-scale models, we investigate the effect of EICP on hydraulic properties in microfluidic experiments by measuring the pressure drop to calculate the permeability and by observing the pore-space alterations with optical microscopy. The experimental setup and procedure is described in [2]. The results of the current study show that under continuous flow conditions and ongoing precipitation preferential flow paths are forming. Our aim is to analyze this effect of strong local inhomogeneity for REV-scale permeability. We expect to quantify this as anisotropy also in pore-scale numerical investigations based on the images obtained from optical microscopy.

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Time Block A (09:00-12:00 CET) **References:**

Hommel, J., Coltman, E., Class, H.: Porosity-Permeability Relations for Evolving Pore Space: A Review with a Focus on (Bio-)geochemically Altered Porous Media. *Transport in Porous Media* (2018), 124 (2), 589-629.

Weinhardt, F., Class, H., Vahid Dastjerdi, S., Karadimitriou, N., Lee, D., Steeb, H. Experimental Methods and Imaging for Enzymatically Induced Calcite Precipitation in a microfluidic cell. Accepted in *Water Resources Research* (2021). **Acceptance of Terms and Conditions:**

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**Poster + / 477**

## The effect of void structure on the permeability of fibrous networks

**Authors:** Antti Koponen<sup>1</sup>; Axel Ekman<sup>None</sup>; Keijo Mattila<sup>None</sup>; Ahmad Al-Qararah<sup>None</sup>; Jussi Timonen<sup>None</sup>

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A Kozeny-Carman based model of permeability is extended by incorporating information about the local structure of the void space. Furthermore, it is demonstrated how this added structural information can be retrieved from a three-dimensional digital image of a porous material. The proposed model is validated with both foam- and water-deposited high-porosity laboratory sheets made of CTMP and Kraft fibers. The validation is carried out by comparing the model predictions against computationally determined permeability values. The related fluid flow simulations are executed using the lattice-Boltzmann method together with high-resolution X-ray microtomography images. The proposed model is shown to improve prediction of permeability for the fibrous materials considered: the deviation between the predicted and computationally determined values is no more than 8%.

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**MS2 / 559**

## The impact of drought-induced root and root hair shrinkage on root-soil contact

**Author:** Patrick Duddek<sup>1</sup>

**Co-authors:** Mutez Ahmed<sup>2</sup>; Nicolai Koebernick<sup>3</sup>; Luise Ohmann<sup>4</sup>; Goran Lovric<sup>5</sup>; Andrea Carminati<sup>1</sup>

<sup>1</sup> *ETH Zurich, Physics of Soils and Terrestrial Ecosystems*

<sup>2</sup> *University of Bayreuth, Soil Physics*

<sup>3</sup> *Martin Luther University Halle-Wittenberg, Soil Science and Soil Protection*

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Increasing the contact area between roots and soil, root hairs are hypothesized to be a key plant strategy facilitating nutrient and root water uptake. Although future agriculture will have to deal with an increasing water and nutrient deficiency, there is still a lack of knowledge regarding root responses to soil drying. In particular, the effect of drought stress on root-soil contact remains unknown. Hence, the objective of our study was to determine morphological responses of roots and root hairs to soil drying in situ.

For this purpose, we have grown maize plants (*Zea mays* L.) in 3D-printed seedling holder microcosms. After a growing period of 8 days, plants were harvested and scanned using a synchrotron radiation CT in order to visualize root compartments as well as the elongated root hairs. The obtained images served as a basis for both image analysis and numerical modelling.

The results revealed that not only roots but also root hairs lose turgidity under dry soil conditions. Root hair shrinkage occurs at high soil water potentials and leads to a severe reduction of both the surface area and the soil contact area of roots. It represents the first step in a sequence of responses to progressive soil drying, followed by the formation of cortical lacunae and root shrinkage. The latter results in air filled gaps at the root-soil interface and thus in a further loss of contact to the soil. Only minor cavitation within the xylem was observed at the corresponding soil water potentials meaning that xylem embolism occurs at even lower potentials.

The data suggest that there is a tremendous loss of root-soil contact and consequently of hydraulic conductivity at the root-soil interface before xylem cavitates and reduces water as well as nutrient fluxes in the axial root direction. Although it is not yet clear if shrunk root hairs are inactive in nutrient and water uptake, their enormous shrinkage due to soil drying might limit rhizosphere processes.

Additionally, we estimated the importance of root hairs on root water uptake by means of image-based simulation of water flow through soil and roots, explicitly accounting for pore scale features such as: root hairs, root-soil matrix contact and air-filled gaps at the root-soil interface and within the root tissue.

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MS6-A / 68

## The impact of pore scale complexity on fluid invasion patterns in heterogeneous rocks

**Authors:** Tom Bultreys<sup>1</sup> ; Arjen Mascini<sup>2</sup> ; Shan Wang<sup>1</sup> ; Sharon Ellman<sup>1</sup> ; Leo Ruspini<sup>3</sup> ; Marijn Boone<sup>4</sup> ; Veerle Cnudde<sup>1</sup>

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Multiphase flow in porous rocks plays a crucial role in CO<sub>2</sub> sequestration, subsurface energy storage and aquifer remediation. The main missing link in understanding the physics of this process is the transition from the length and time scales of a single pore to those of a macroscopic description. At

the intermediate scale, intricate fluid distribution patterns emerge, closely tied to the geometry and surface chemistry of the pore space. Starting with Lenormand et al's seminal work, there has been significant progress in classifying the invasion patterns in model porous media based on e.g. the capillary number, viscosity ratio and contact angle<sup>1–3</sup>. However, it remains unclear how this translates to multi-scale, heterogeneous pore spaces typically found in geological reservoirs. We hypothesize that strong pore-scale variability in the viscous-capillary force balance may yield qualitatively new behavior in such cases. This is corroborated by fluid invasion experiments in rock samples imaged by fast micro-computed tomography. We discuss recent advances in multi-scale pore network modelling and wettability characterization to explain and classify the observed phenomena. The developed methods aim to establish a solid basis to explore when, where and why different fluid distributions occur; providing a valuable starting point to improve large-scale modelling of subsurface engineering projects.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

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MS6-A / 379

## The impact of roughness and wettability on imbibition in a fracture

**Authors:** Yu Qiu<sup>None</sup>; Ke Xu<sup>1</sup>; Amir Pahlavan<sup>2</sup>; Ruben Juanes<sup>3</sup>

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Understanding the physics of immiscible fluid-fluid displacement in fractures is central to many applications, including hydrocarbon recovery, groundwater contamination by nonaqueous liquids, and geologic CO<sub>2</sub> sequestration. Much of the experimental research on fluid-fluid displacement has focused on smooth fractures and, as a result, the hydrodynamic impact of roughness, especially under unfavorable viscosity contrast and in strong imbibition, remains to be better understood.

Here, we experimentally investigate forced imbibition under unfavorable viscosity contrast (water displacing viscous silicone oil) in a microfluidic fracture, which is a modified Hele-Shaw cell with one plate patterned with a regular honeycomb array of cylindrical posts. This setup allows us to precisely control the fracture aperture, roughness and wettability. We investigate the impact of four parameters: (1) fracture aperture (gap thickness between two plates); (2) roughness amplitude (post height); (3) contact angle of water immersed in silicon oil ( $\theta$ ); and (4) capillary number.

Our experimental system allows us to visualize the fluid displacement patterns that develop on the plane of the fracture, and also—by means of a carefully determined calibration curve—the fluid distribution across the gap. We find three types of invasion paths: (1) water completely fills the channel including both the gap space and roughness crevices, which we term “complete displacement”; (2)

water preferentially invades along the roughness as a “thick film”, where water covers the rough surface; (3) water preferentially invades within the roughness as a “thin film”. Such “thin film” invasion makes the dynamics of imbibition in a rough fracture substantially distinct from that in a smooth cell 1.

These invasion paths together lead to different regimes of imbibition displacements, the transitions between which are explained by the interplay among capillarity and viscous effects in the gap space and the roughness. “Thin film” may occur only when the equilibrium contact angle is below a critical threshold ( $\theta_c$ ), in which the energetic cost of displacement within the roughness is always negative. This is an analogue of the hemi-wicking regime in an unconfined system [2]. However, in a rough confined system, the balance between capillary pressure within the roughness and across the gap space further determines the imbibition configurations at low capillary number: if the roughness capillarity dominates, we observe wicking into roughness; while if gap capillarity dominates, water adopts “complete displacement”, but with finger width decreasing to around one pore unit. Further, at high capillary number, liquid entrainment is triggered in the three-phase contact line, with the wetting phase preferentially advancing ahead of the bulk water. If  $\theta > \theta_c$ , the preferential path is a “thick film”, like the forced imbibition pattern on smooth fractures 1, while if  $\theta < \theta_c$ , the roughness provides an extra preferential “thin film” flow path.

We propose a phase diagram that delineates the different regimes of imbibition dynamics, which explains our experimental data quantitatively. In particular, it includes a novel pattern of forced imbibition in a rough fracture controlled by a “thin film” fluid-displacement mechanism—a finding that challenges the current description and modeling of fluid-fluid displacement in fractured media.

#### Time Block Preference:

Time Block C (18:00-21:00 CET) **References:**

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MS2 / 311

## The importance of accurate evapotranspiration forecast for crop irrigation: A global sensitivity analysis of two model case studies

**Authors:** Theodor Bughici<sup>1</sup> ; Naftali Lazarovitch<sup>2</sup> ; Eran Tas<sup>3</sup>

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A reliable forecast of potential evapotranspiration ( $ET_0$ ) and precipitation can be used for precision crop irrigation. A multi-objective evolutionary algorithm (MOEA) optimization followed by a sensitivity analysis (SA) of a crop model (HYDRUS-1D) for two case studies was performed in order to assess the crop model sensitivity to weather forecast accuracy. A  $\pm 5\%$  of  $ET_0$  relative bias range was found to be a threshold for  $ET_0$  forecast accuracy being a non-dominant parameter for both spring potatoes growing in loamy sand and summer peanuts growing in silty clay. For both case

studies soil hydraulic parameters dominated model output and increased with increasing  $ET_0$  forecast accuracy. With respect to model output of actual transpiration, maximum root depth was also dominant for the first case study and although precipitation for the test cases was scarce, the rainfall bias parameter dominated excess drainage of water and solutes. This MOEA–SA scheme for crop model analysis can help set priorities in irrigation management by ranking the data that is most important to be accurately determined in order to optimize crop production.

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## The influence of surfactant flooding on oil displacement in Nano-Silica Pores

**Authors:** Wei Yong<sup>1</sup> ; Jos Derksen<sup>1</sup> ; Yingfang Zhou<sup>1</sup>

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Surfactant flooding has considered to be one of the most useful approach to recovery residual oil that trapped in pore space after waterflooding. From a macroscopic perspective, this is the surfactant molecules – that are adsorbed on the oil/water interface – would significantly reduce the interfacial tension (IFT) and thus result in the change of wettability in the oil-water reservoir system. However, the microscopic mechanism of surfactant structure (the hydrophilic headgroup and the hydrophobic hydrocarbon chain) effecting on IFT and contact angle is still lack of deep investigation. In the present study, we performed a detailed molecular dynamics (MD) simulation (all the simulations are conducted with the open-source MD code - LAMMPS) study to understand the displacement and transportation of oil droplets in nanopores with surfactant solution interactions at the atomic levels. We first demonstrated the surfactant molecules forming micelle process in a water environment and then revealed the mechanism of two factors (interfacial thickness and interface formation energy) effecting on surfactant-IFT reduction as well as the temperature sensitivity with respect to IFT. Related results are consistent with previous simulation and experimental work (Palazzesi et al., 2011; Xu et al., 2013). The surfactant molecules have been further added into water/oil system to investigate the influence of surfactant flooding on oil droplet displacement and transportations. Liquids/silica pore surface wettability associated with the surfactant additions is evaluated by the contact angle of oil droplet at the three-phase contact line.

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## The morphology and surface-chemistry of gas-wetting nanoparticles and its effect on the liquid menisci in porous media

**Authors:** Jin Jiafeng<sup>1</sup> ; Sun Jinsheng<sup>1</sup> ; Lv Kaihe<sup>1</sup>

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The transformation of the liquid menisci at pore throats is of great importance for mitigating the liquid-blocking effect of condensate reservoirs. Here, we reported a super gas-wetting peanut-like nanoparticle which can facilitate the liquid menisci to transform from concave-shape to convex-shape by coating a super gas-wetting adsorption with high surface roughness. The morphology and surface chemistry of gas-wetting nanoparticles were investigated by SEM, AFM, and XPS analysis. The mechanism of surface modification was further explored by TEM, the adsorption layer coated on the nanoparticle surface can be recognized as monolayer adsorption. Gas-wetting model is recommended as the combination of the Wenzel model and Cassie-Baxter model, which is in close agreement with the results of AFM and Contact-angle measurement. Core flooding visualization was performed to identify the effect of gas-wetting alteration on the transformation of liquid menisci in porous media. Results showed that the addition of gas-wetting nanoparticles could decrease the liquid saturations by inducing the transformation of liquid menisci in the pore throat. Additionally, a unique "Amoeba effect" and miscibility effect can synergistically improve the mobility of the oil phase, further enhance the oil recovery.

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MS21 / 163

## The relevance of simple probabilistic models for deposition, accumulation and transport of colloidal particles proved by real time, internal observations (MRI, confocal microscopy)

**Authors:** Philippe Coussot<sup>1</sup> ; Philippe Coussot<sup>2</sup>

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Colloidal particles from industrial or natural sources propagate and may deposit and alter the environment they flow through. Predicting particle transport and deposition in these porous media is key to solve these problems. Deposition models generally propose empirical corrections of the common advection/diffusion system of equations to take into account the different types of interactions between the particles and the solid walls of the porous structure, generally through a modification of the adsorption kinetic constant. However, the validity of these approaches is often only indirectly tested through the analysis of the breakthrough curve, corresponding to the exited concentration as a function of time.

Here we review the conclusions of a series of experiments [1-4] with model materials in which it was possible to observe directly the deposit, possible accumulation, or transport of the colloidal particles



inside the material. The internal observations are carried out thanks to confocal microscopy or Magnetic Resonance Imaging measurements. The results tend to show that whatever the mechanism of deposition (size exclusion effect or bridging, adsorption on pore walls, aggregation with other particles) rather simple models taking into account a deposition probability are sufficient to describe the whole process of transient deposition and transport throughout the sample. This in particular makes it possible to show that the propagation of particles takes the form of travelling waves <sup>1</sup>. It is also shown that similar approach with now two different probabilities can be appropriate to describe the transport and deposition properties in more complex media with two pore sizes <sup>1</sup>.

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[2] N. Bizmark, J. Schneider, R.D. Priestley, S.S. Datta, Multiscale dynamics of colloidal deposition and erosion in porous media, *Sciences Advances*, 6, eabc2530 (2020)

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1 G. Gerber, D. A. Weitz, and P. Coussot, Propagation and adsorption of nanoparticles in porous medium as traveling waves, *Phys. Rev. Research* 2, 033074 (2020)

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MS20 / 482

## The role of collateral vessels in redistributing blood flow during stroke – combining in vivo data with blood flow simulations in semi-realistic networks using an inverse model

**Authors:** Robert Epp<sup>1</sup> ; Nadine F Binder<sup>2</sup> ; Chaim Glück<sup>3</sup> ; Mohamad El Amki<sup>2</sup> ; Susanne Wegener<sup>2</sup> ; Bruno Weber<sup>3</sup> ; Patrick Jenny<sup>None</sup> ; Franca Schmid<sup>4</sup>

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Due to the limited energy storage capabilities of the brain, maintaining a robust oxygen and nutrient supply to all regions of the brain is crucial. During healthy conditions, the interconnected network of blood vessels sustains blood flow to all brain areas. However, during stroke the overall blood supply is reduced drastically. This typically causes tissue damage, which often results in permanent disability or even death.

Generally, the microvasculature of the brain cortex consists of three vessel categories: (1) the surface vessels, (2) the penetrating trees and (3) the capillary bed. Collaterals are blood vessels connecting major feeding arteries at the surface of the brain, e.g. the middle and anterior cerebral arteries (MCA, ACA). If the primary flow path is blocked due to occlusion of the MCA, collaterals provide an alternative route for blood to partially maintain perfusion in the under-supplied brain region (MCA region). Therefore, vascular networks with collaterals are more robust towards tissue damage during stroke

[El Amki & Wegener (2017)].

The goal of our work is to better understand the role of collaterals in redistributing flow during stroke and during the subsequent recanalization of the occluded vessel. To date, blood flow can only be quantified in a small number of vessels, hence in vivo measurements only provide limited insight on overall changes in perfusion and on the role of the collaterals. Consequently, we employ numerical simulations [Schmid et al. (2017)] to compute flow and pressure characteristics in large semi-realistic microvascular networks. Here, we present a novel approach to generate such networks by combining realistic arterial networks with an artificial capillary bed. To achieve diameter and flow rate distributions consistent with sparse in vivo measurements, the diameters of the entire network are adjusted by solving an inverse problem using the adjoint method [Epp et al. (2020)]. This allows us to generate large microvascular networks which (a) represent the structure of the real vasculature and (b) are consistent with in vivo measurements in individual subjects with and without collaterals. Our results confirm that the reduction of overall perfusion after MCA occlusion is less severe in networks with collaterals. Moreover, we show that the redistribution of flow is a direct consequence of the pressure changes initiated by the occlusion and occurs even without collateral dilation. This results in a substantial increase in flow in all collaterals and in the majority of surface arteries at the ACA side, as well as a directed flow from the ACA- towards the MCA-supplied territory.

In summary, our approach allows to incorporate sparse experimental data into blood flow simulations. This strengthens the link between in vivo and in silico studies and allows quantitative and combined study designs. The developed simulation framework enables us to study transient changes during treatment as well as the role of changes at the capillary level during stroke. Both aspects are highly relevant for the recovery of the patient but difficult to study in vivo.

#### Time Block Preference:

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## Theoretical analysis of poroelastic response of spherical indentation into a half space via step-displacement loading

**Author:** Haiying Huang<sup>1</sup>

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The process of indentation by a rigid tool has been widely studied for its versatility as an experimental technique to probe constitutive properties of materials of various kinds across multiple scales. Recently the technique has been applied to characterize poroelasticity of soft materials such as polymeric gels via load relaxation experiments, where an indenter is pressed instantaneously to a fixed depth and held until the indentation force approaches a horizontal asymptote. Assuming incompressibility in both the solid and fluid phases, elastic constants are determined from the early and late time responses, while the hydraulic diffusivity is obtained from the transient response by matching the

experimentally obtained indentation force as a function of time against a master curve obtained from FEM simulations 1. The numerical analysis assumes a negligible effect of the Poisson's ratio and a mixed drainage surface condition where the area underneath the indenter is impermeable while the region outside is fully drained.

Motivated by these experimental advances in soft materials, we analyze indentation of a poroelastic solid by a spherical-tip tool within the framework of Biot's theory. The McNamee-Gibson displacement function method is employed to solve the cases where the indenter is subjected to a step displacement loading. Three types of surface drainage conditions, namely, fully drained, fully undrained and mixed drainage, are analyzed. Compressibility of both the fluid and solid phases is considered in these solutions. Though derivation of these theoretical solutions requires the aid of a variety of mathematical techniques to overcome the difficulties related to integrals with rapidly oscillating kernels and solving the Fredholm integral equation of the second kind, the results in terms of the normalized indentation force relaxation with time are remarkably simple. The transient force responses show only weak dependence on one derived material constant and can be fitted by elementary functions, which lend themselves to convenient use for material characterization in the laboratory.

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Time Block C (18:00-21:00 CET) **References:**

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MS1 / 632

## Thermal fracturing and natural convection – a hidden source of geothermal activity in the earth's crust?

**Authors:** Sæunn Halldorsdottir<sup>1</sup> ; Inga Berre<sup>1</sup> ; Eirik Keilegavlen<sup>1</sup> ; Ivar Stefansson<sup>1</sup> ; Gudni Axelsson<sup>2</sup>

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We consider fracture propagation driven by cooling that is mainly caused by convection cells inside vertical fractures. The process, known as convective downward migration, has been proposed as a mechanism for transport of heat in the deep roots of volcanic geothermal systems. It is also predicted to have an important role in the source mechanism of hydrothermal activity in a more general perspective. In a numerical study, the PorePy code is applied to model these coupled THM processes. With the focus on convection-driven cooling, where natural fluid convection induces thermo-poromechanical stress changes leading to fracture deformation and propagation in a single vertical fracture. We identify parameters affecting this natural phenomenon and investigate how these are controlled by regional and local settings; perhaps explain existence of geothermal systems in some locations over others. We explain the concept of "hidden geothermal systems" and discuss how knowledge of thermal fracturing and natural convection can facilitate for broader utilization of enhanced geothermal systems in locations where regional settings might not favor natural hydrothermal systems.

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MS6-A / 541

## Thermodynamic Stability of Bubble Population in Porous Media

**Authors:** Ke Xu<sup>1</sup> ; Yashar Mehmani<sup>2</sup> ; Chuanxi Wang<sup>1</sup> ; Yuehongjiang Yu<sup>1</sup>

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Bubbles (or droplets, ganglia) emerge in porous media aftermath of flow, phase change, or chemical reactions and significantly impact the hydraulic, transport, and reactive properties of the system. However, compared to continuously connected phases, the behavior of dispersed bubbles, or ganglia, are far less understood. In particular, the thermodynamic stability of bubbles, despite their large specific surface area, remains a puzzle.

Our earlier works (Xu et al., PRL, 2017; Xu et al., GRL, 2019; Mehmani et al., in preparation) have shown that bubble population in porous media can keep stable, rather than coarsen like bubbles in open space, by “anti-coarsening”. This anti-coarsening is shown to be driven by Ostwald ripening as that in open space, but the driving force – capillary pressure difference – is reversed by porous structure. Further pore-network modelling (PNM) approach show distinct ripening kinetics of bubbles in porous media from Classic L-S-W theory.

However, these above approaches only demonstrate one kinetic mechanism that stabilizes the bubble population, without answering the very fundamental question: is the bubble population in a porous medium thermodynamically stable? The answer would be very important to interpret the origin and long-term evolution of dispersed fluids in subsurface porous media, which is highly relevant to geologic CO<sub>2</sub> sequestration, hydrocarbon recovery, fuel-cell water management, and vadose zone oxygen supply.

To identify bubble population’s thermodynamic stability in porous media, we propose a simple conceptual model in 2-dimensional (2D) to describe the equilibrium states of a bubble with arbitrary size inside a homogeneous porous medium. The model accounts for the bubble’s morphology, the geometry of the solid matrix, and the wettability between the two, and enable an analytical expression of a bubble’ capillary pressure ( $P_c$ ) and surface free energy ( $F$ ) as functions of bubble volume ( $V$ ), bubble Euler characteristic ( $X$ ), and pore occupancy ( $n$ ). This model can be easily incorporated into PNM approaches.

This conceptual model shows that, when a bubble is larger than the maximum inscribed sphere of a pore, it starts to be deformed by porous structure, and both  $P_c$  and  $F$ ’s scaling against  $V$  deviate from that for spherical bubbles. Specifically, the specific area of a large bubble (spanning over more than one pore) fluctuates in a very narrow interval regardless of  $V$ , which results in an approximately linear correlation between  $F$  and  $V$  regardless of the ( $X, n$ ) value. As a result, merging of bubbles does not necessarily reduce total free energy, so bubble coalescence and coarsening become thermodynamically unfavorable.

Therefore, we demonstrate that bubble populations in porous media can be thermodynamic stable, without continuously coarsening towards the formation of one single big bubble. We further calculate the total free energy of a bubble population and identify all possible final equilibrium status of bubble population. Future study will focus on extend this conclusion to more complex scenario, like non-uniform pore size and 3D scenario.

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## Three-Dimensional Imaging of Density-Driven Convection in Porous Media Using X-ray CT Scanning

**Author:** Anna-Maria Eckel<sup>None</sup>

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In the context of subsurface CO<sub>2</sub> storage, the mixing process is triggered by the local density increase in the ambient brine following the dissolution of CO<sub>2</sub>. As a result, gravitational instabilities occur and characteristic, perpendicular elongated finger-like patterns form that are enhancing the mixing between CO<sub>2</sub> and water compared to a purely diffusive process. This density-driven mixing process is considered as a key trapping mechanism for subsurface CO<sub>2</sub> storage, because it accelerates the dissolution of CO<sub>2</sub> into brine and could eventually form a stable stratification in the aquifer, thereby reducing the chances of leakage.

Owing to the difficulty of imaging the time-dependent convective process, experiments so far have largely focused on two-dimensional systems (e.g., Hele-Shaw cells). However, the convective fingers are propagating into all three spatial directions and neglecting the third spatial dimension imposes a strong restriction on the lateral spreading of the plumes. To explore the dynamic flow pattern within a three-dimensional medium, we developed an experimental procedure by applying X-ray CT imaging and 3D reconstructions that allow visualisation of the evolution of the plumes non-invasively at a high spatial and temporal resolution. To imitate the dissolution process of CO<sub>2</sub> in brine under laboratory conditions, we use salt with a high X-ray attenuation coefficient that dissolves in water and creates a heavier solution than pure water. We perform dissolution experiments for a range of Rayleigh numbers and infer several global quantities including the average mass fraction, dissolution flux and dilution index. We show that the three-dimensional mixing evolves successively through three regimes, starting with a simple one-dimensional diffusional profile, transit into a convection-dominated regime and continues to attain the maximum dissolution capacity of the system with the shutdown.

Results provide more representative information towards the investigation of convective mixing in the context of Carbon Capture and Storage. Insights into the complex three-dimensional mixing structures will additionally support the elucidation if two-dimensional scaling laws can successfully predict three-dimensional behaviour.

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## Threshold pressure for the capillary with irregular cross section

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Threshold pressure (or capillary entry pressure) is the minimum pressure difference required for the non-wetting fluid to penetrate a capillary filled with a wetting fluid. It is well known that this capillary pressure for the circular capillary can be calculated by Young-Laplace equation. While for capillaries with irregular sections, the MS-P method, which was originally proposed by Mayer and Stowe (1965) and further developed by Princen (1969a, 1969b, 1970), has been widely used to analytically estimate the threshold pressure. However, the equations derived from MS-P method are very complicated and unconcise.

In this work, we derivate a concise and accurate predictor of the threshold pressure in irregular capillaries using the Reduced Similar Geometry (RSG) method (Mason and Morrow,1991), which is a special case of the MS-P method. The main idea of the RSG method is to remove the central portion of cross section occupied by the non-wetting phase and construct a reduced cross section shape similar to the original. First, we extend the RSG method to tangential polygons. Then we simplify the threshold pressure equation into a concise form by introduce a completeness factor. This factor indicates the completeness of the inscribed circle in the reduced shape and is decided by the shape factor and wetting conditions. Further, we generalize this concise equation to capillaries with arbitrary cross sections by changing the completeness factor. The short explanation is for the proposed equation is that the threshold radius is the weighted harmonic mean of the maximum inner circle radius and area equivalent radius (the square root of the ratio of area to  $\pi$ ). This study can help understand the capillary behavior better and provide a fast tool to predict the threshold pressure in irregular capillaries.

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## To biofilm or not to biofilm: Interplay between chemotactic dispersal and biofilm formation in bacterial communities

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**Co-authors:** Daniel Amchin<sup>1</sup> ; Selena Chiu<sup>1</sup> ; Tapomoy Bhattacharjee<sup>2</sup> ; Sujit Datta<sup>3</sup>

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Bacteria are ubiquitous in our daily life, frequently as surface-attached biofilm communities. In some cases, biofilms serve a positive purpose, such as improving health or remediating polluted water; in other cases, they negatively impact our lives, such as by causing infection or fouling equipment. For both positive and negative purposes, understanding the factors that regulate the onset of biofilm formation is crucial in determining how to control or treat them. However, how bacteria transition between the free-swimming planktonic state to the sedentary biofilm state in these heterogeneous environments is poorly understood. Here, we use computational modeling to investigate how biofilm formation depends on bacterial properties as well as the properties of their environment. Specifically, by analyzing the competition between chemotactic dispersal and quorum sensing, we establish universal rules predicting how the onset and extent of biofilm formation depend on cell concentration and motility, nutrient diffusion and consumption, chemotactic sensing, and autoinducer secretion. The findings from this study therefore yield quantitative principles to predict biofilm formation.

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## Toolchain from the creation of the mesh to the CFD simulations

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**Co-authors:** Yann Henry ; Jean Bouyer ; Pascal Jolly ; Pascal Doumalin ; Aurelian Fatu ; Anthony Beaudoin ; Endri Lacaj

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The performance of many industrial applications is largely based on the quality and reliability of the guidance and support systems (high rotational speeds, low friction torque, damping capability, etc.). The subject presented here is part of an ANR project, entitled SOFITT (Saturated Open-pore Foams for Innovative Tribology in Turbomachinery) and aiming to find innovative technical solutions that break with current practices and provide high-performance support systems in terms of load capacity and damping. The project proposes a new concept of lubrication and correspondingly a new material (understood as a complex/composite material formed by the solid porous structure - compressible porous layers - and the imbibing fluid) in order to improve the quality and reliability of the guidance and supporting systems. The CFD (Computational Fluid Dynamics) simulations offer an economical solution to study the performance of this new concept of lubrication. The main objective is to understand the behavior of the porous complex structures, linked to microstructural properties of the solid material and their interactions with the fluid. In the scientific literature, the works studying the flow in compressible materials are essentially experimental because of their very complex geometrical shape 1, [2], [3]. The work proposed in this paper is a current challenge in the scientific community. The difficulty in performing CFD (Computational Fluid Dynamics) simulations in porous materials is to access the geometry of their structure. Thus, a first task is devoted to the simulation at the microscopic scale of the flow through a porous medium. The morphological structure of polyurethane foam samples is reconstructed at different levels of compression from 3D X-ray microtomography. This is achieved by using a commercial software (Avizo) that allows to

process 3D images and create FE/CFD models suitable for numerical analysis [4], [5]. A procedure allowing the passage between the microtomography measurements and the numerical models is developed. Then CFD modelling allows to study the impact of the material deformation on the pressure drop correlations [6], [7]. The numerical models are validated with experimental measurements conducted previously and presented in the reference [8].

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

- 1 S. Dasa, S. Sneijdersa, N.G. Deenb and J.A.M. Kuipersa, Drag and heat transfer closures for realistic numerically generated random open-cell solid foams using an immersed boundary method, *Chemical Engineering Science*, 183, pp. 260-274, 2018.
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**Poster + / 159**

## Tortuosity and permeability of random porous medium using deep learning

**Authors:** Maciej Matyka<sup>1</sup> ; Krzysztof Graczyk<sup>1</sup>

<sup>1</sup> *Faculty of Physics and Astronomy, University of Wrocław*

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We will present our recent results on porosity (P), permeability (K), and tortuosity (T) of artificial, randomly generated porous medium predicted directly from the geometry images 1. We will show that convolutional neural networks (CNN) can predict porosity, permeability, and tortuosity based only on the obstacles' picture. The CNN is trained on artificial data samples, for which the permeability and tortuosity are obtained within the Lattice-Boltzmann method. The CNN predicts permeability and tortuosity with about 6% accuracy.

1 Graczyk, K. M., and Matyka, M., Predicting Porosity, Permeability, and Tortuosity of Porous Media from Images by Deep Learning, *Sci Rep* 10, 21488 (2020)

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Graczyk, K. M., and Matyka, M., Predicting Porosity, Permeability, and Tortuosity of Porous Media from Images by Deep Learning, *Sci Rep* 10, 21488 (2020) **Acceptance of Terms and Conditions:**



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MS1 / 71

## **Towards Geologic CO<sub>2</sub> Sequestration at Scale: A Review of Geomechanical Impacts, Induced Seismicity Concerns, and Mitigation Measure**

**Authors:** Jens Birkholzer<sup>1</sup> ; Yves Guglielmi<sup>1</sup> ; Keurfon Luu<sup>1</sup> ; Jonny Rutqvist<sup>1</sup> ; Abdullah Cihan<sup>1</sup>

<sup>1</sup> *Lawrence Berkeley National Laboratory*

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After decades of research on carbon capture and geologic sequestration (CCS), the world needs to finally move from pilot and demonstration experiments to industrial-scale implementation. CCS at scale will involve unprecedented fluid injection volumes that can result in large-scale pressure increases in the subsurface and may cause unwanted geomechanical effects, such as generating seismic events per reactivation of critically stressed faults. Understanding and predicting induced seismicity potential is critical in CCS projects for two reasons: (1) to avoid the potential for damaging earthquakes at the ground surface, and (2) to ensure that caprock integrity is not jeopardized by permeability increases of slipping faults. Also, in a future world with CCS being a fully deployed technology, sedimentary basins with interconnected reservoirs might host multiple storage sites between which pressure interference can be expected. Thus, large-scale pressure buildup can be a limiting factor for CO<sub>2</sub> sequestration capacity, because of induced seismicity concerns or because the possibility of distant pressure-related impacts of individual projects needs to be considered. It has been pointed out that the subsurface storage capacity for CO<sub>2</sub> may be increased via extraction of the native brines, a pressure management approach that of course comes with additional cost for the handling, treatment or disposal of the extracted brine and thus needs to be carefully optimized.

This presentation will start with a short description of the current worldwide status of CCS and its role as an important climate-mitigation technology. We will then illustrate the basin-scale pressure impacts expected from industrial-scale implementation based on regional modeling studies of future CCS scenarios, and will discuss the potential for generating earthquakes from CCS at scale using the practice of waste water injection in Oklahoma and surrounding States in the U.S. as an analog. We will also present lessons learned from two field experiments—one being a controlled-injection fault slip experiment in a clay (caprock) formation which is highlighting the importance of aseismic leakage and its potential coupling to induced seismicity, the other a CO<sub>2</sub> demonstration site where micro-seismicity has occurred along pre-existing basement faults—and will finally evaluate brine extraction as a mitigation measure currently tested in a deep reservoir in the southern United States.

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## **Towards HPC simulations of Billion-cell Reservoirs by Multiscale Mixed Methods**

**Authors:** Roberto Ausas<sup>1</sup> ; Alfredo Jaramillo<sup>2</sup> ; Rafael T. Guiraldello<sup>3</sup> ; Stevens Paz<sup>None</sup> ; Fabricio Sousa<sup>1</sup> ; Felipe Pereira<sup>4</sup> ; Gustavo Buscaglia<sup>1</sup>

<sup>1</sup> *University of Sao Paulo*

<sup>2</sup> *USP, Brazil*

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<sup>4</sup> *Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA*

**Corresponding Authors:** rfausas@icmc.usp.br, luisfelipe.pereira@utdallas.edu, stevens2221@gmail.com, trevi@usp.br, ajaramillopalma@gmail.com, fsimeoni@icmc.usp.br, gustavo.buscaglia@icmc.usp.br

A three dimensional parallel implementation of Multiscale Mixed Methods based on non-overlapping domain decomposition is proposed and its computational performance is assessed by means of numerical experiments. As a prototypical method the Multiscale Robin Coupled Method 1 is chosen and its implementation is explained in detail. Numerical results for problems ranging from millions up to more than 2 billion computational cells in highly heterogeneous anisotropic rock formations based on the SPE10 benchmark [2] are shown. The proposed implementation relies on direct solvers for both the local problems and the interface coupling system. It exhibits good weak and strong scalability as compared against a state-of-the-art global fine grid solver based on Algebraic Multi-grid preconditioning [3] in single and two-phase flow problems.

**Keywords:** Porous media, Darcy's law, Two-phase flow, High Performance Computing, Multiscale method, Domain Decomposition

**Time Block Preference:**

Time Block C (18:00-21:00 CET) **References:**

1 R. T. Guiraldello, R. F. Ausas, F. S. Sousa, F. Pereira, and G. C. Buscaglia. The multiscale Robin coupled method for flows in porous media. *Journal of Computational Physics*, 355:1–21, 2018.

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MS9 / 487

## **Towards Unified Pore-Scale Imaging and Modelling: Comparison of the Generalized Network Model with Direct Numerical Simulation**

**Author:** Luke Giudici<sup>1</sup>

**Co-authors:** Ali Qaseminejad Raeini<sup>2</sup> ; Martin Blunt<sup>3</sup> ; Takashi Akai<sup>3</sup> ; Branko Bijeljic<sup>1</sup>

<sup>1</sup> *Imperial College*

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**Corresponding Authors:** a.qaseminejad-raeini09@imperial.ac.uk, lp2815@ic.ac.uk, m.blunt@imperial.ac.uk, akai-takashi@jogmec.go.jp, b.bijeljic@imperial.ac.uk

A thorough understanding of pore-scale modelling techniques is essential to flow through permeable media research. We compare two phase-flow simulations from the generalised network model (GNM) [Raeini et al, 2017, 2018] with a recently developed lattice-Boltzmann model (LBM) [Akai et al, 2018, 2020] for drainage and waterflooding in two samples – a synthetic beadpack and a micro-CT imaged Bentheimer sandstone – for water-wet, mixed-wet and oil-wet states. We further compare

the GNM to a volume-of-fluid method [Shams et al. 2018] for two-phase flow in a synthetic two-pore system. An analysis of macroscopic capillary pressure shows a large discrepancy between the GNM and both direct numerical simulations, with volume-of-fluid simulations highlighting the need for accurate pore-space geometry in network modelling. Pore-by-pore comparison between the GNM and LBM reveals a good agreement for oil and water-wet media. The comparison for mixed-wet media, however, shows greater differences. We suggest that the dependence of displacement on wettability in the mixed-wet state is responsible for this discrepancy. Compared to the LBM, the GNM can reach lower initial water saturations and captures the effect of layer flow — a prohibitively expensive task for LBMs — by achieving a lower residual oil saturation after waterflooding in altered wetting states. Overall, we present a workflow for the comparison of porenetwork models with direct numerical simulation of multi-phase flow. We demonstrate their strengths and shortcomings through an analysis of local and macroscopic parameters while showing how high-fidelity approaches can be used to facilitate future network model development.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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Akai, T., Lin, Q., Bijeljic, B., and Blunt, M. J. (2018). Wetting boundary condition for the color-gradient lattice Boltzmann method: Validation with analytical and experimental data. *Advances in Water Resources*, 116:56–66

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Poster + / 566

## Towards bottom-up design of porous electrode microstructures - coupling genetic algorithms with pore network modeling of redox flow battery electrodes

**Author:** Maxime van der Heijden<sup>1</sup>

**Co-authors:** Rik van Gorp<sup>1</sup>; Gabor Szendrei<sup>1</sup>; Amin Sadeghi<sup>2</sup>; Jeffrey Gostick<sup>2</sup>; Zandrie Borneman<sup>1</sup>; Antoni Forner-Cuenca<sup>3</sup>

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Integrating renewable energy technologies into the grid is necessary to enable a sustainable energy economy but is currently challenged by their intrinsic intermittency. Redox flow batteries (RFBs) are rechargeable electrochemical reactors that are promising for grid-level energy storage due to their ability to decouple energy and power. However, current RFB systems remain too costly for widespread deployment<sup>1</sup>. Porous electrodes are performance-defining components as they must facilitate mass transport, provide surfaces for electrochemical reactions, and conduct electrons and heat. Thus, optimizing the porous electrode microstructure offers a promising pathway to cost reduction by increasing power density [2], [3]. Traditional, empirical design of electrodes is time- and

resource-intensive and does not enable exploration of the wider design space but is currently limited to carbonaceous fibrous structures. To accelerate progress, microstructure-informed multiphysics simulations (e.g. pore network modeling, lattice Boltzmann) can be leveraged to aid the theoretical understanding and design of advanced electrode architectures but has been limited to exploration of existing, carbon-fiber based electrodes [4]–[6]. In this work, we explore the following scientific question: *Can we deploy three-dimensional simulations in combination with evolutionary algorithms to enable artificial generation of electrodes from the bottom-up?*

In the first part of this talk, the modeling framework will be introduced. We developed a microstructure-informed, electrolyte-agnostic electrochemical pore network model (PNM) integrated in an open access platform (OpenPNM) [6], [7]. The model was validated using a symmetric flow cell for two distinct electrolytes (an aqueous  $\text{Fe}^{2+}/\text{Fe}^{3+}$  and a non-aqueous TEMPO./TEMPO+) and two types of porous electrodes (a carbon paper -Freudenberg H23- and a carbon cloth -ELAT Cloth-). The dry electrode microstructure was obtained with x-ray computed tomography and converted into a network of spherical pores and cylindrical throats using the SNOW algorithm [8]. The electrochemical model is solved for the electrolyte fluid transport, species transport, and charge transport with low computational cost (123,335 pores, 60-120 min on an Intel® Core(TM) i7-8750H CPU). For the non-aqueous electrolyte, the model accurately predicts the electrochemical performance without fitting parameters, allowing rapid benchmarking of porous electrode microstructures in a time-efficient manner. For the aqueous electrolyte, we find that incomplete wetting of the electrode results in overprediction of the electrochemical model that assumes one-phase flow and employ thermal pretreatment to demonstrate the importance of complete wetting on the modeling validation [9]. Fitting of the near-surface mass transfer coefficient enables accurate representation of the experimental data. Finally, the PNM framework was coupled with a genetic algorithm based on Darwin's evolutionary theory that is used to perform artificial generation of porous electrodes for RFBs from the bottom-up. With this method, chemistry-specific electrode architectures can be optimized based on the electrolyte properties alone.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

- 1 R. M. Darling, K. G. Gallagher, J. A. Kowalski, S. Ha, and F. R. Brushett, "Pathways to low-cost electrochemical energy storage: A comparison of aqueous and nonaqueous flow batteries," *Energy Environ. Sci.*, vol. 7, no. 11, pp. 3459–3477, 2014.
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## Towards scalable multi-scale open-source solvers for ionic trans-

## port and electrochemistry

**Authors:** Robert Barnett<sup>1</sup> ; Matteo Icardi<sup>1</sup> ; Federico Municchi<sup>None</sup> ; John King<sup>1</sup>

<sup>1</sup> *University of Nottingham*

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In this work we present open-source solvers, based on the finite volume library OpenFOAM, for solving the Stokes-Poisson-Nernst-Planck (SPNP) system of equations for single or multi-domain ionic transfer. Many applications that involve said ionic transport, e.g reinforced concrete [1], batteries [3] and oil extraction [2], also involve heterogeneous reactions between domains. As such, interface conditions have been formulated and implemented to model this mass exchange between ionic species.

After outlining the governing equations, a dimensional analysis will be presented to note the various transport regimes capable of being seen under different scenarios by quantifying ratios between transport phenomena. We then discuss the features and capabilities of the pore-scale solvers (pnpFoam and pnpMultiFoam), as well as the heterogeneous reactive conditions (mappedChemicalKinetics). These solvers and conditions will then be verified under different test cases by comparing results against high-order spectral results obtained with the MatLab toolbox Chebfun. Since a large number of applications of SPNP involve complex porous geometries (e.g., batteries involve a porous solid electrode flooded with fluid electrolyte), we consider the case of two- and three-dimensional randomly generated porous domain of solid and fluid [5]. Preliminary results will be presented to determine the set of geometrical parameters, through uncertainty quantification, that have significant effect on the ionic transport.

Solving at the microscale over complex porous mediums involving large scales seen in many applications is computationally intensive. Later work will be outlined to accommodate this by formulating homogenized models, parametrising the geometrical complexity, and developing therefore novel macroscopic model suitable for dominant reaction and fast ionic transfer regimes [4].

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MS25 / 95

## Transdisciplinary Soil Hydrology

**Author:** Jan Jan W Hopmans<sup>1</sup>

<sup>1</sup> *University of California Davis*

**Corresponding Author:** jwhopmans@ucdavis.edu

Using an evolutionary pathway from disciplinary towards transdisciplinary science and research, I explore exciting opportunities that can lead to transdisciplinary research as society demands for our science expertise to be increasingly involved in developing solutions for global issues of sustainability. I do this by presenting excellent examples by way Dr. Harry Vereecken has taken this challenging path. Recommendations are presented to better train students and early-career scientists so that they can be effective in participating and communicating their scientific knowledge to relevant stakeholders, the public, and decision makers when being part of the policy-making process.

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(MS25) Subsurface Water Flow and Contaminant Transport Processes – Special Session in Honor of Harry Vereecken **Acceptance of Terms and Conditions:**

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## Transient ground water level simulation scale with pre-calculated time-varying recharge values

**Authors:** Diederik Jacques<sup>1</sup> ; Bertrand Leterme<sup>1</sup> ; Matej Gedeon<sup>1</sup>

<sup>1</sup> *SCK CEN*

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The recharge from the soil to the groundwater is a crucial variable to simulate time-variable groundwater levels and gradients at a catchment scale. Although essential for groundwater modelling, no direct measurement methods are available. One way to estimate this variable is to calculate it from time-series of atmospheric boundary conditions (precipitation, potential evaporation) for specific soil types, land uses, and ground water depths. In this study, we pre-calculated monthly and seasonally recharge rates as a function of three parameters for an area in Northern Belgium. Soil type and land use were inferred from geographic information systems. Soil hydraulic properties were derived from soil textural information for a soil information system (AARDEWERK) using pedotransfer functions. Vegetation parameters were taken from the literature. Recharge values were calculated using the HYDRUS-1D model with time-series of daily atmospheric input data for a period of 20 y. A series of models were ran for each soil-type/land use combinations with the fixed groundwater level type bottom boundary with depth in a range between 5 and 200 cm. Next, monthly recharge values were obtained for the complete period for each calculated ground water level. In additions, a future climate time series of atmospheric input data was obtained by applying monthly correction factors derived from a regional climate model (Ntegeka et al., 2008). Resulting look-up table with soil-type, land-use and groundwater depth combinations served as an input to a MODFLOW model recharge (RCH) and evapotranspiration (EVT) package to simulate transient ground water levels and fluxes at the current and future climate. We shortly discuss our MCMC calibration to ground water level and fluxes, validation and water budgets for current and future climate conditions.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

Ntegeka V., Baguis P., Boukhris O., Willems P., Roulin E., 2008. "Climate change impact on hydrological extremes along rivers and urban drainage systems. II. Study of rainfall and ETo climate change scenarios", Belgian Science Policy – SSD Research Programme, Technical report CCI-HYDR project by K.U.Leuven – Hydraulics Section & Royal Meteorological Institute of Belgium, May 2008, 112 p **Acceptance of Terms and Conditions:**

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## Transport analysis in deformable porous media through integral transforms

**Authors:** Alessandra Bonazzi<sup>1</sup> ; Birendra Jha<sup>1</sup> ; Felipe P. J. de Barros<sup>1</sup>

<sup>1</sup> *University of Southern California*

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Geomechanical deformation can alter the flow field which impacts solute mass fluxes. Despite its importance, the effects of the coupling between geomechanical deformation and the flow field on solute transport behavior are not fully known. In this work, we study the impact of this coupling on the solute concentration distribution. The concentration field is semi-analytically derived by making use of the Generalized Integral Transform Technique. We apply the semi-analytical solution to two uniaxial consolidation problems, the classical Terzaghi's problem with a constant load and the case of periodic loading of a porous deformable layer. Our results indicate that geomechanical parameters, such as the Skempton's coefficient and the soil compressibility, can affect the peak concentration as well as the spatial moments of solute plume. In case of periodic loading, we show that the frequency of loading also plays a key role in regulating the temporal dynamics of the concentration field.

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## Transport of chemotactic bacteria in porous media with residual sources of chemical pollutants

**Author:** Roseanne Ford<sup>None</sup>

**Corresponding Author:** rmf3f@virginia.edu

Nonaqueous phase liquid (NAPL) contaminants are difficult to eliminate from natural aquifers due, in part, to the heterogeneous structure of the soil matrix. Residual NAPL ganglia remain trapped in regions where the hydraulic conductivity is relatively low and they are consequently less bioavailable. Bioremediation processes depend on adequate mixing of microbial populations and the groundwater contaminants that they degrade. The ability of chemotactic bacteria to sense a chemical gradient and swim preferentially up the gradient toward higher concentration can enhance the accumulation of bacteria near contaminant sources that may otherwise not be readily accessible by advection and dispersion alone.

In this work, we directly imaged *Pseudomonas putida* bacteria near naphthalene sources trapped within a pore network etched into a microfluidic device. We modeled bacterial transport at the pore scale using a convection-dispersion equation with the addition of chemotactic velocity to the convective term and first-order sorption-desorption kinetics for retention around NAPL ganglia. Previous simulations at the core scale in granular media showed that the heterogeneous hotspots of

chemotactic bacteria around NAPL ganglia yielded overall greater retention of biomass in breakthrough curves compared to a nonchemotactic control. Our experimental observations at the pore scale confirmed the core scale simulation results by revealing greater accumulation of chemotactic bacteria (relative to a nonchemotactic control) near ganglia of naphthalene sources. Our pore scale simulation results showed that greater retention of bacteria was due to its chemotactic response to naphthalene gradients and sorption to NAPL ganglia. Our modeling predictions in combination with laboratory experiments at varying scales can be a useful tool to analyze the impact of chemotaxis on in situ bioremediation. This work is in collaboration with Xiaopu Wang, (China University of Petroleum-East China) and Beibei Gao (University of Virginia).

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## Transport properties modelled on multiscale porous media images

**Author:** Iman Nabipour<sup>1</sup>

**Co-authors:** Jafar Qajar<sup>2</sup> ; Hamed Aghaei<sup>3</sup>

<sup>1</sup> *PhD Student of Petroleum Engineering, Department of Petroleum Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz, Iran*

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Carbonate rocks are characterized by their complicated and heterogeneous pore structure [1]. In general, mechanical and chemical compaction, cementation, dissolution, mineral transformation and fracturing are among the most important factors typically affecting the fabric of a carbonate rock, and so, its lithofacies and petrophysical properties (e.g. porosity and permeability) [2]. In this case, a detailed knowledge of pore scale geometry is inevitable for a deeper understanding from the physics of fluid flow and transport through such a porous media. In recent years, emergence of the non-invasive micro-computed tomography ( $\mu$ CT) technique has made it possible to visualize the internal structure of porous materials [3-5]. However, quantification of pore scale heterogeneities depends largely on sample size and detector specifications. In other words, despite a larger volume of the samples can be imaged in a low resolution imaging, in which are more representative of a typical heterogeneous sample, but more microstructural details can be lost due to partial volume effect which in turn limits the direct simulation of transport processes [6, 7]. The primary aim of this work is to present an image processing and computational workflow for predicting absolute permeability in low-resolution images of selective carbonate samples that are too large to allow direct simulation. After acquisition of  $\mu$ CT images with different spatial resolutions on a tight carbonate rock sample, the workflow involves direct pore scale simulation of permeability by the Lattice-Boltzmann method in a high-resolution image, together with a number of geometrical and topological characteristics obtained from spatially registered lower resolution images of the same sample. In addition, a machine learning technique was developed based on Convolutional Neural Networks (CNNs) to correlate the parameters obtained from low-resolution images to the ones driven from higher resolution images. Note that a texture interpolation technique was employed for the purpose of data augmentation between images acquired at different scales. The results of CNN modelling confirmed the permeability values estimated from lower resolution images for which high-resolution images are needed for direct simulation.

**Time Block Preference:**



Time Block A (09:00-12:00 CET) **References:**

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MS3 / 760

## Transport-Related Consequences of Geochemical Interactions between Shale, Formation Brine, and Reactive Fluid

**Authors:** Asli S. Gundogar<sup>1</sup> ; Cynthia M. Ross<sup>1</sup> ; Jennifer L. Druhan<sup>2</sup> ; Adam D. Jew<sup>3</sup> ; John R. Bargar<sup>3</sup> ; Anthony R. Kavscek<sup>1</sup>

<sup>1</sup> *Stanford University*

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The complex interplay of injected reactive fluid with shale minerals and resident formation brine has a potentially significant role in the rapid decline of hydrocarbon production following fracturing operations. A sudden inflow of reactive fluid into brine-bearing shales that are initially in equilibrium causes mineral dissolution and precipitation reactions. These reactions contribute dramatically to reaction-induced porosity and permeability reductions. Elucidating fracture fluid behavior in shale systems is crucially important for reducing environmental impacts by reusing water, prolonging recovery, and thereby improving sustainability. In this study, the influence of shale-mixing fluid interactions on flow properties was examined by means of representative core-flooding experiments and multiscale imaging tools. The study samples, cored parallel to bedding planes (2.54-cm diameter and ~7.6-cm length), were selected from the economically critical U.S. shale resources, namely Marcellus, and Wolfcamp plays with their diverse structural and mineralogical backgrounds. Basin-specific formulas (Marcellus and Midland) were used for brine and HCl-based fracture fluid (pH=2) solutions. In the flow experiments, brine and fracture fluid were injected sequentially under confining stress (up to 500 psi) at reservoir temperature (80°C). Reaction-related mineralogical, structural, and petrophysical alterations were investigated using X-ray diffraction, medical computed tomography (CT), microCT, scanning electron microscopy (SEM)-energy dispersive spectrometry (EDS), and pulse-decay permeability methods. Importantly, inductively coupled plasma - optical emission spectrometry/mass spectrometry (ICP-OES/MS) tool was utilized to probe chemical composition evolution of the core-flood effluents. Krypton flooding tests were conducted under in-situ X-ray CT

that enables the pre-/post-reaction spatial and temporal evolutions in Kr-accessible porosity distributions within the shales. CT-number distributions under totally vacuum states that are directly proportional to shale density revealed dissolution and scale precipitation paths across the core samples. Mineral reactions in response to acidic fluid reduced system porosity and core permeability. SEM-EDS results showed significant iron hydroxide precipitates in clay- and pyrite-rich samples due to partial oxidation of iron-bearing phases. Porosity reductions in carbonate-rich samples are related to compaction of cores under stress due to matrix softening with dissolution, and pore-filling by Fe, Al, and Mg-Al hydroxides, as well as barite and salts. ICP tests revealed time-resolved concentration trends in produced brine and reactive fluids that in turn complemented SEM-EDS based observations. The greatest release of metals to brines was in clay-rich systems indicating the importance of equilibrium between shale and synthetic brine prior to reactive fluid exposure. Based on reactive flow experiments, formation water in shales, mixing of brine with fracture fluid during flow, and shale mineralogy have a significant impact on scale precipitation. Experimental data was employed to calibrate transport modeling of reactive fluids and to reproduce the results of aqueous and kinetic reactions identified by SEM-EDS and ICP data. Reactive flow at approximate to reservoir conditions provides a critical basis for evaluating coupling between transport and geochemical processes and correlating the outcomes to the field conditions.

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MS12 / 463

## **Two-grid coupled multiphase flow and geomechanics: A computational framework to monitor surface deformation along with fault slip due to pore pressure perturbations**

**Author:** Saumik Dana<sup>1</sup>

**Co-author:** Birendra Jha<sup>1</sup>

<sup>1</sup> *University of Southern California*

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We develop a computational framework that leverages the features of sophisticated software tools and numerics to tackle some of the pressing issues in the realm of earth sciences. The algorithms to handle the physics of multiphase flow, concomitant geomechanics and the complex geometries of field cases with surfaces of discontinuity are stacked on top of each other in a modular fashion which allows for easy use to the end user. The current focus of the framework is to provide the user with tools for assessing seismic risks associated with energy technologies and for estimating properties in the subsurface as they evolve real-time.

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Poster + / 359

## Two-scale poromechanical model incorporating adsorption effects of a fluid mixture in arbitrary geometrical nanopores

**Authors:** Quoc Dat HA<sup>1</sup> ; Tien Dung LE<sup>1</sup> ; Irina Panfilov<sup>1</sup> ; Christian Moyne<sup>1</sup>

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A two-scale poromechanical model incorporating the complex adsorption phenomena of a fluid mixture in nanopores is developed in this work. The porous medium is composed of a solid phase and nanopores of size of several nanometers where adsorption occurs. The adsorption isotherm of a fluid mixture is rigorously constructed by using the Density Functional Theory (DFT) and the Fundamental Measure Theory (FMT) [1,2] applied to a Lennard-Jones fluid. It should be noted that the studies in the literature have been limited to the case of slit, cylindrical or spherical pores [3,4,5] in which the problem can be reduced to one dimension and analytical solutions can be derived. In our work, a novel numerical method based on the Fast Fourier Transform (FFT) and 3D-voxel discretization is developed to accurately compute the fluid mixture density distributions in an arbitrary geometrical pore in three dimensions. The pore domain is firstly discretized by voxels of the same size. In this configuration, the convolution terms can be solved in Fourier space giving a huge advantage in terms of time calculation and computer resources. Numerical simulations show the density profiles of CH<sub>4</sub> and CO<sub>2</sub> gas mixture in an ellipsoidal pore, considering the fluid-fluid and solid-fluid Lennard-Jones interaction-types, highlighting the potential of the current method. Such approach is capable of computing accurately the adsorbed gas densities in any pore geometry, regardless of the difference of molecule diameters.

Given the gas densities, the solvation force, which is the force exerting on the solid wall by the fluid phase in arbitrary geometrical nanopores, is then computed by using a new derived formulation obtained from mechanics and thermodynamics approaches. It is important to notice that the solvation force in the pore is normally negative and its order of magnitude is much higher than the bulk pressure, leading to an important impact on the mechanical properties at higher scale. To consider this force in the poromechanical model, the local mechanical description at the pore scale is upscaled to the macroscale by using the homogenization technique in the sense of [4,5]. As a result, the macroscopic total stress tensor is the sum of a classical elastic part and a solvation component due to the solvation force which acts as a pre-stress inside the material. This analysis allows accurately predicting the volumetric strain of the medium with respect to variation in pressure and gas composition. Numerical simulations show an application to coalbed methane, predicting the coal matrix swelling with the increase in gas pressure. It is highlighted that the adsorption potential of CO<sub>2</sub> is higher than the one of CH<sub>4</sub>, therefore the volumetric strain due to the increase in CO<sub>2</sub> pressure is much more significant.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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## Uncertainty Quantification of Relative Permeability Measurements by Inverse Modelling

**Authors:** Steffen Berg<sup>1</sup> ; Evren Unsal<sup>1</sup> ; Harm Dijk<sup>1</sup>

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Multiphase flow in porous media plays a key role for many energy-related processes, ranging from transport in gas diffusion layers in fuel cells to the recovery of oil and gas from subsurface geological formations. Uncertainty assessment of e.g. hydrocarbon recover processes is typically performed on the basis of field-scale flow simulations which use a continuum mechanics formulation based on Darcy's law and phenomenologically extended to multiphase flow. One of the consequences of that phenomenological extension is the introduction of empirical parameters such as the relative permeability-saturation function which need to be determined experimentally. The field-scale model predictions have a very high sensitivity on the uncertainty in the relative permeability-saturation functions. Therefore, it is important to understand the uncertainty of relative permeability associated with the experimental measurements and data interpretation.

Relative permeability is obtained by interpreting production, saturation data and pressure drop from flow experiments by either analytical methods or inverse modelling. Traditionally, inverse modelling is performed by manually which does not provide a systematic estimate of the associated uncertainty. We have developed a framework for a consistent uncertainty assessment of relative permeability measurements. Inverse modelling is automated using the Python optimization toolbox coupled a flow simulator. Either conventional flow simulation packages such as reservoir simulators are coupled with a wrapper, or a native Python implementation is used which is a factor 400 faster. That allows to go beyond the gradient-based optimization approaches but apply a Markov-chain Monte Carlo (MCMC) scheme on 10 or more parameters within an acceptable time.

We find in practically all cases considered signature of non-uniqueness, which can be suppressed by involving more and different types of data, e.g. saturation profiles but not fully eliminated. By matching the flow model directly to the data provides significantly smaller uncertainty ranges than first performing a manual match and then fitting the resulting tabulated relative permeability with an analytical function. Due to the phenomenological history of the 2-phase Darcy approach, it is furthermore not clear which parameterization for relative permeability should be used. By comparing a Corey with a LET representation we see better consistency with the data using the LET function, but still residuals have non-Gaussian structure, suggesting that current models are not a fully adequate representation of the experimental reality, which calls for a more in-depth understanding of the flow experiments und underlying flow regimes.

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Poster + / 454

## Uncertainty-aware Validation Benchmarks for Coupling Free Flow and Porous-Medium Flow

**Author:** Farid Mohammadi<sup>1</sup>

**Co-authors:** Bernd Flemisch<sup>2</sup> ; Sergey Oladyshkin<sup>2</sup> ; Elissa Eggenweiler<sup>2</sup> ; Iryna Rybak<sup>2</sup> ; Kilian Weishaupt<sup>2</sup> ; Martin Schneider<sup>2</sup>

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A correct choice of interface conditions and useful model parameters for coupled free-flow and porous-medium systems is vital for physically consistent modeling and accurate numerical simulations of applications. We consider the Stokes-Darcy problem with different coupling strategies: classical and generalized interface conditions on the sharp fluid-porous interface and the pore-network model. The classical set of interface conditions is the most widely used coupling concept in the literature; however, it contains several uncertain parameters. We quantify these uncertainties and study the coupled flow problem's behavior considering several benchmark cases, where the pore-scale resolved model is used as the reference solution. The coupled Stokes-Darcy model with the classical set of interface conditions is also validated by comparing the pore-network model and the recently developed generalized interface conditions. All the model parameters are computed based on the pore geometry.

We apply a statistical framework that incorporates a probabilistic modeling technique using a fully Bayesian approach to accomplish these goals. A Bayesian perspective on a validation task yields an optimal bias-variance trade-off against the reference data. It provides an integrative metric for model validation that incorporates parameter and conceptual uncertainty. Additionally, a model reduction technique, namely Bayesian Sparse Polynomial Chaos Expansion, is employed to accelerate the calibration and validation processes for computationally demanding models for Stokes-Darcy problem with different coupling strategies. We perform uncertainty aware validation, demonstrate each model's predictive capabilities, and make a model comparison using Bayesian validation metrics.

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## **Under pressure: Hydrogel swelling in a granular medium**

**Authors:** Jean-Francois Louf<sup>1</sup> ; Nancy Lu<sup>1</sup> ; Margaret O'Connell<sup>1</sup> ; H. Jeremy Cho<sup>1</sup> ; Sujit Datta<sup>2</sup>

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Hydrogels hold promise in agriculture as reservoirs of water in dry soil, potentially alleviating the burden of irrigation. However, confinement in soil can markedly reduce the ability of hydrogels to absorb water and swell, limiting their widespread adoption. Unfortunately, the underlying reason remains unknown. Here, we report the first direct visualization of hydrogel swelling within a model three-dimensional (3D) granular medium with tunable confining stresses and grain sizes. Our experiments enable us to measure, *in situ*, two key quantities that were previously inaccessible: the extent of hydrogel swelling and medium restructuring. Unlike an imposed osmotic or hydrostatic pressure, confinement in a granular medium subjects the surface of a hydrogel to a spatially nonuniform stress. We therefore extend the classic Flory-Rehner theory of hydrogel swelling by coupling it to Hertzian contact mechanics that explicitly treats the stresses exerted by the medium at the hydrogel-grain contacts. Using this approach, we show that the extent of hydrogel swelling is determined by the balance between the osmotic swelling force exerted by the hydrogel and the confining force transmitted by the surrounding grains. Furthermore, we demonstrate that a balance of the same forces, also including intergrain friction, determines the onset of restructuring of the surrounding medium. Our work therefore reveals the physical principles that describe how hydrogel swelling in and restructuring of a granular medium both depend on the properties of the hydrogel, the properties of the medium, and confining stress. We show that our theoretical framework not only describes our

measurements but also helps to rationalize previous measurements of hydrogel water absorption in soil. Together, our results provide quantitative principles to predict how hydrogels behave in confinement, potentially improving their use in agriculture as well as informing other applications such as oil recovery, construction, mechanobiology, and filtration.

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Under pressure: Hydrogel swelling in a granular medium  
J-F Louf, N. B. Lu, M. G. O'Connell, H. J. Cho, S. S. Datta, *Science Advances*, 7, eabd2711 (2021)  
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## Underground Hydrogen Storage: a multiscale experimental-numerical study

**Author:** Hadi Hajibeygi<sup>1</sup><sup>1</sup> *TU Delft***Corresponding Author:** h.hajibeygi@tudelft.nl

Subsurface geological formations provide giant capacities for storing renewable energy, when it is converted into green gas (e.g. hydrogen) or compressed and hot fluids. While the utilisation of subsurface formations have a long track of success in the past decades, their successful contribution in the energy transition towards a green world comes with new scientific challenges. The cyclically-stored fluids are expected not only to be stored safely, but to be reclaimed efficiently and with the same purity as in the injection phase. The critical stress also will impose restrictions on the volume, rate, and frequency of the storage cycles. In this talk, I will introduce this topic to the Interpore scientific community, and describe its key ingredients. Then a comprehensive multiscale lab-model development is presented. Objectives are to characterize the cyclic hysteretic fluid transport and rock mechanics across scales in variety of rocks from salt caverns to heterogeneous fractured porous media.

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MS19 / 470

## Understanding Electrolyte Infilling for Lithium Ion Batteries

**Authors:** Christina Sauter<sup>1</sup>; Raphael Zahn<sup>1</sup>**Co-author:** Vanessa Wood<sup>1</sup><sup>1</sup> *ETH Zurich*

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Lithium ion batteries consist of three main porous components: anode, cathode and an electronically isolating membrane in between. This so-called separator prevents physical contact between the two electrodes while the pore space is filled with electrolyte to allow ionic transport. Therefore, the separator is considered to be a crucial part in battery safety.<sup>1</sup> Filling of the electrode and the separator with an electrolyte is a crucial and time-consuming step in the lithium ion battery manufacturing process and incomplete filling negatively impacts electrochemical performance, cycle life, and safety of cells.

Our research group has developed an approach to visualize and quantify a polyethylene (PE) separator with focused ion beam scanning electron microscopy (FIB-SEM).<sup>[2,3]</sup> The so-obtained 3D structure is used as a model system for typical polyolefin lithium ion battery separators, since it consists of a single solid phase with relatively uniform pore size and isotropic pore structure.

The 3D data set allows us to simulate the wetting of the separator membranes with liquid electrolyte. We perform quasi-static infilling simulations on the separator and show that during this imbibition-process up to 30% gas is entrapped in the separator. Using partial wetting theory, we show that the specific pore structure of the separator is responsible for this incomplete wetting.

A traditional parameter to characterize the performance of a separator is the effective transport coefficient (ratio between tortuosity and porosity). This value can be experimentally measured by electrical impedance spectroscopy (EIS).

Comparing the wetting simulations to these separator performance measurements, we demonstrate, that incomplete wetting can explain the discrepancy between theoretically predicted and experimentally measured transport coefficients. We also show that quasi-static wetting models overestimate the amount of residual gas in the membranes and that realistic wetting models have to consider both, the physio-chemical properties of the liquid electrolyte and the 3D structure of the separator pore space. Our work highlights the importance of pore structure in determining the amount of residual gas in a structure and provides insights into the pore structures, infilling conditions, and electrolyte formulations that are advantageous for battery technology.<sup>[4]</sup>

#### Time Block Preference:

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## Understanding dynamic pore-scale interactions for underground hydrogen storage through high resolution 3D X-ray imaging

**Authors:** Zaid Jangda<sup>1</sup> ; Kamaljit Singh<sup>1</sup> ; Sebastian Geiger<sup>None</sup> ; Andreas Busch<sup>1</sup>

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Reducing the carbon footprint and the commitment to achieve net-zero targets will be the drivers of global environmental and energy policies in the years to come. Clean energy sources could soon become the premium choice for power generation and transportation. Hydrogen is an important clean and promising alternate energy option that is growing rapidly. Blue hydrogen is made from natural gas through the process of steam methane reforming coupled with CCS, while green hydrogen is produced from water using renewable power. Especially for the latter, there can be a mismatch between production and consumption, requiring intermittent storage in periods of low energy demand, that can be utilized in periods of high energy demand. Clean hydrogen can be stored in large volumes in underground formations, such as salt caverns, depleted hydrocarbon reservoirs and saline aquifers.

Although storage of gas in underground reservoirs has been vastly studied and implemented for natural gas and to a certain extent CO<sub>2</sub>, hydrogen storage poses its unique challenges due to its distinctive physical and chemical properties. Hydrogen is more prone to microbiological reactions, has a higher diffusivity and mobility and can have several chemical interactions with the subsurface fluids and rock formations, especially in the presence of clays. All these factors need to be considered before designing an underground hydrogen storage facility. Limited data is available on the feasibility of underground storage of hydrogen for extended periods of time and pore-scale interactions with reservoir fluids and rocks is still not well understood as there are no studies conducted to visualize or observe these interactions.

Recent advances in X-ray  $\mu$ CT to image multiphase flow in porous media and perform in-situ measurements, has allowed to visually observe and quantify the complex pore-scale displacement events occurring under reservoir conditions. These images and measurements have contributed enormously to developing the correct strategies for hydrocarbon recoveries and CO<sub>2</sub> storage, and to comprehend the interactions between multiple reservoir fluids at different conditions.

Aiming to achieve a similar level of insight for hydrogen storage, this study discusses pore-scale imaging experiments to capture the interaction between hydrogen, reservoir fluids and rocks. These experiments allow us to visualize the flow patterns as hydrogen is injected into the porous rock in the presence of brine, and to measure in-situ contact angles ascertaining the wettability at different points in porous media. Understanding the interactions between hydrogen and brine can be the first step towards designing an underground hydrogen storage facility in aquifers or depleted hydrocarbon reservoirs. Our research aims to provide an initial indication about the trapping mechanisms and therefore storage efficiency that will occur when large scale hydrogen injection is implemented on the field-scale level. Further research is planned to understand these interactions under different pressure, temperature, and salinity conditions, and using different flow parameters.

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## **Understanding the combined effect of structural and wettability heterogeneity on two-phase flow in porous media**

**Author:** Amir Jahanbakhsh<sup>1</sup>

**Co-authors:** Omid Shahrokhi<sup>1</sup> ; Mercedes Maroto-Valer<sup>1</sup>

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The individual and combined impact of pore size disorder and wettability on the fluid distribution in different applications including hydrocarbons recovery, underground storage and soil remediation has been widely studied [1,2]. However, the combined effect of heterogeneities in both pore structure and wettability is not fully understood. Wettability plays an important role in multiphase flow which is generally classified as homogeneous and heterogeneous (also known as fractional and mixed) [3,4,5]. Unlike homogeneous wettability, where the whole rock surface has a uniform molecular affinity to the fluids in contact, for heterogeneously wetted porous media there is a variation in affinities for the fluids at different regions [5]. Moreover, most rocks naturally have a propensity to display heterogeneous wettability due to their formation diagenesis.

Limited pore-scale experimental studies (e.g. micromodel testing) have been performed on microscale wettability heterogeneity mainly due to fabrication challenges [3,6]. Significant impact on fluid displacement and level of residual saturation have been observed in porous media with non-uniform wettability [3]. Fabricating a large number of porous media replicas with different spatial configurations for wettability heterogeneities may not be feasible, and therefore, using pore-scale numerical simulation can provide insights into multiphase flow and trapping for different scenarios and optimize further experimental investigation. However, to the best of our knowledge, most of the published numerical simulation studies have investigated the effect of different homogenous wettability on fluid flow dynamics in either homogenous or heterogeneous pore structure.

In this work, we have used direct numerical simulations (DNS) to investigate wettability and structural heterogeneity at pore-scale. DNS studies were conducted using the Phase Field method and commercial computational fluid dynamics (CFD) software (COMSOL Multiphysics) [7]. We have built Quasi-3D pore-scale models and simulated two-phase flow in porous media. Two-phase flow displacements are compared at different uniform and non-uniform contact angle distributions for homogenous and heterogeneous porous structures. We systematically change the pore structure heterogeneity in the pattern to better understand the combined effects of wettability and structural heterogeneities.

We observed that non-uniform wettability distribution is as important as structural heterogeneity and their combined effect has a significant impact on the evolution of fluid interface, displacement efficiency and trapped saturation. Simulations showed that trapped saturations can be either continuous or discontinuous based on the imposed spatial configuration of wettability on the heterogeneous media. Certain wettability configurations, e.g. being parallel to the flow direction, promote flow instability for the same pore-scale geometry, while others, such as being perpendicular to the flow direction, may assist the front stability and result in less trapping. The results of these DNS studies are of interest to different subsurface processes involving reactive transport and wettability alteration.

#### **Acknowledgement**

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (MILEPOST, Grant agreement no.: 695070). This paper reflects only the authors' view and ERC is not responsible for any use that may be made of the information it contains.

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Time Block A (09:00-12:00 CET) **References:**

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## Understanding the influence of pore-scale rock heterogeneity in CO<sub>2</sub> geo-sequestration

**Author:** Farshad Daraei Ghadikolaei<sup>1</sup>

**Co-authors:** Yulai Zhang<sup>2</sup>; Lydia Knuefing<sup>2</sup>; Anna Herring<sup>3</sup>; Mark Knackstedt<sup>4</sup>; Mohammad Saadatfar<sup>5</sup>

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Subsurface storage of CO<sub>2</sub> involves the injection of CO<sub>2</sub> into suitable geological formations and the monitoring of the injected plume over time. The science and technology of CO<sub>2</sub> geo-sequestration has been maturing over the last two decades. To increase the effectiveness of the underground CO<sub>2</sub> sequestration, the multi-phase-flow and its relevant mechanisms that change the distribution and concentration of the underground CO<sub>2</sub> must be assessed at multiple lengths scales. Predicting the behavior of CO<sub>2</sub>-brine in the complex heterogeneous porous structure of reservoir rocks as well as the interaction between these fluids with minerals in rocks are important for designing and managing CO<sub>2</sub> storage sites.

In this work, we present lab-based experimental studies of CO<sub>2</sub>-brine-rock systems at subsurface conditions. We use x-ray micro-CT to map the distribution of fluids in heterogeneous sandstone rocks. Our work combines experimental, 3D and 4D imaging and image analysis of simulated geo-sequestration of CO<sub>2</sub> conditions. We provide experimental and numerical analysis that shed light on the role of rock heterogeneity on the safety and capacity of CO<sub>2</sub> geo-sequestration at the pore scale.

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## Understanding the mechanisms of the brain's waterscape

**Author:** Marie E. Rognes<sup>1</sup>

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Your brain has its own waterscape: whether you are reading or sleeping, fluid flows around or through the brain tissue and clears waste in the process. These physiological processes are crucial for the well-being of the brain. In spite of their importance we understand them but little. Mathematics and numerics could play a crucial role in gaining new insight. Indeed, medical doctors express an urgent need for modeling of water transport through the brain, to overcome limitations in traditional techniques. Surprisingly little attention has been paid to the mechanisms and the numerics of the brain's waterscape however, and even fundamental knowledge is missing.

In this talk, we will look at mathematical, mechanical and numerical aspects for understanding mechanisms involved in the brain's waterscape across scales. At the macroscale, the brain can be viewed as a poroelastic medium with multiple fluid and pressure compartments interacting. At the mesoscale, the vasculature twist and turn through the brain parenchyma: defining lower dimensional structures interacting with the brain tissue. And at the microscale, brain cells and extracellular space interact via electrical, chemical and mechanical signalling.

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## Unified multiphysics framework for assessment of CO<sub>2</sub> storage in heterogeneous saline aquifers

**Authors:** Yuhang Wang<sup>1</sup> ; Cornelis Vuik<sup>1</sup> ; Hadi Hajibeygi<sup>2</sup>

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CO<sub>2</sub> injection into deep saline aquifers has shown to be a feasible option in many locations in the world, as for their large storage capacity under safe operational conditions. Previous studies have revealed that CO<sub>2</sub> can be trapped in the subsurface by several mechanisms, including hydrodynamical, residual, dissolution, and mineral trapping. Despite the major advances in studying these trapping mechanisms, their dynamic interactions have been widely ignored; i.e., they are studied independently at their so-called 'separated time scale of importance'. These mechanisms, however, are dynamically interconnected and influence each other even outside of their main time scale of importance. Specially in presence of heterogeneous rock properties and complex CO<sub>2</sub>-brine thermo-hydraulic interactions, it is not trivial to assume these trapping processes have separation of scales in the time domain. Of great importance is to quantify the interactions between different trapping mechanisms, and allow for a fully-coupled multiphysics strategy in estimations of the trapped mass. To this end, we present a full-cycle coupled multiphysics workflow, in which the CO<sub>2</sub> injection, migration and post-migration processes are all considered in a unified multiscale-in-time framework. Our framework specially represents hysteresis characteristics of the constitutive Kr and Pc relations. Moreover, a compositional formulation representing a two-component, two-phase system is employed to capture dissolution trapping at all time. Note that dissolution is often times studied much longer after injection. However, as a significant step forward, we include all of these physics, including dissolution, at all times. As for a convenient implementation strategy, we utilized the well-developed black-oil-type formulation, where only the lighter component (CO<sub>2</sub>) exists in both phases. In particular, the CO<sub>2</sub>-brine ratio (similar to the solution gas-oil ratio) is calculated based on a thermodynamic model which are verified against experimental measurements. The overall-composition variable set is used and the coupled system is solved using a fully implicit scheme; allowing for a robust coupling treatment.

Through several test cases, we quantify the impact of different trapping mechanisms and uncertain reservoir and fluids parameters on the injection, migration and post-migration of CO<sub>2</sub>. We demonstrate that the time scale associated with each trapping mechanism indeed varies significantly, yet

their dynamic interplay needs to be considered for accurate and reliable simulations. Our studies shed new lights on the impact of the coupled reservoir and fluid time-dependent interactions in estimation of the securely trapped CO<sub>2</sub> in the reservoir.

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MS25 / 239

## Unsaturated Flow Effects on Solute Transport in Soils

**Author:** Luwen Zhuang<sup>1</sup>

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A major contaminant transport process in soils is hydrodynamic dispersion by affecting the spreading and arrival of surface-applied pollutants at underlying groundwater reservoirs. When a soil is unsaturated, hydrodynamic dispersion is very much affected by soil water saturation. Centimeter- and decimeter-scale column experiments were carried out to explore the effects of fluid saturation and soil type on the unsaturated solute dispersivity. Measured in-situ breakthrough curves were analyzed in terms of both classical advection-dispersion and dual-porosity (mobile-immobile) type transport equations. A clear non-monotonic relationship was found between the dispersivity and soil water saturation. The extent of non-monotonicity was more pronounced for relatively coarse-textured soils compared to the finer soils. This finding has been reported rarely before; it explains the inconsistency of saturation-dispersivity relationships in the literature. The relationship between solute dispersivity and water saturation proposed herein may improve the performance of field-scale transport models for the unsaturated zone.

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MS25 / 172

## Unsaturated hydraulic properties in a nearly saturated medium

**Author:** John Nimmo<sup>1</sup>

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In models and estimates of unsaturated hydraulic properties, the wet range between field saturation and the air-entry value is greatly oversimplified. Retention curves, for example, are often taken to be perfectly flat (unchanging water content) in this range, or are represented by an empirical formula

that is unrelated to the active processes. Another example is diffusivity, which goes to infinity with a flat retention curve, making it both unrealistic and unusable. Though much neglected, the hydraulic properties of a nearly saturated medium are important in an increasing number of applications, for example:

- Macropore/matrix domain exchange, a major influence on preferential flow processes and control on rapid versus slow solute transport, which often occurs with the matrix domain at high water content.
- The precise timing of the transition from unsaturated to field-saturated conditions, as may be important to initiation of ponding, triggering of landslides, heightened vulnerability to erosion, and initiation of preferential flow.
- Subsurface initiation of preferential flow by seepage from nearly saturated matrix material into macropores.
- Hydraulic property measurement by tension infiltrometer, which frequently is done with the input condition at a very slight suction.

A new process-based model has been developed for the important case of a medium without macropores (i.e. having a distinct nonzero air-entry value) that is exposed to repeated wetting and drying cycles. On wetting, the medium does not exceed field saturation, with trapped air occupying some of the pore space. Water retention in the range between air-entry and field saturation is not dominated by capillarity but by trapped air expansion and contraction with change in matric pressure, and effects triggered by this process. Accordingly, the model represents this wet range by an augmented Boyles' law variation of trapped air volume with matric pressure, amplified by an empirical factor to account for associated liquid-bridge collapse or other mechanisms. Tests using high-quality measurements in this range showed good fits with Boyles' law amplified by a factor typically between 2 and 4.

This model can serve within a model of hydraulic conductivity, treated as saturated conductivity that varies with changes in effective porosity determined by the variable trapped air volume. Diffusivity can then be assigned a realistic value using the modeled retention and conductivity relations. Though few data are available for direct test of these dynamic properties, the model has value for exploring possible consequences of processes occurring under conditions close to field saturation.

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MS17 / 216

## **Unsaturated porous media freezing: numerical modeling and validation based on experimental data**

**Author:** Abdel Hassan Sweidan<sup>None</sup>

**Co-authors:** Yousef Heider<sup>1</sup> ; Bernd Markert<sup>1</sup>

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Ice formation in porous media is a phenomenon characterized by coupled heat and mass transport, which could lead to considerable deformations<sup>1</sup>. Studying such a process is important in many engineering applications. In cold regions where periodic freezing occurs, porous materials like road pavements and concrete are usually subjected to frost damage. Moreover, some techniques such as artificial ground freezing, which are widely used for ground-water control and temporary excavation support, can lead to heave and settlement of the ground surface.

In the underlying work, a numerical modeling framework that takes the multi-physical thermo-hydro-mechanical (THM) processes of ground freezing into account is presented. In this, an unsaturated soil is treated as a non-isothermal, deformable, triphasic porous material with a gas phase and

a single fluid that can change depending on the thermal conditions between a solid ice and a liquid water state. The model is based on a coupled phase-field-porous media approach [2], where the main focus is laid on the temperature-driven processes that lead to the phase transition between water and ice and the freezing-related deformations. The governing equations of the macroscopic model are based on the well-founded theory of porous media (TPM) [3] extended by the phase-field modeling (PFM) [4]. The model proceeds from a small-strains assumption, whereas the pore-fluid can be found in liquid water or solid ice state with a unified kinematics treatment of both states [5]. Comparisons with the experimental data will demonstrate the ability and usefulness of the considered model in describing the freezing of unsaturated soils.

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## Upscaling Inertia Effects on Mixing and Reaction at Channel Intersections from Flow Topology

**Authors:** Peter Kang<sup>1</sup> ; Sang Lee<sup>None</sup> ; Woonghee Lee<sup>2</sup> ; Etienne Bresciani<sup>None</sup> ; Marco Dentz<sup>3</sup>

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<sup>3</sup> *IDAEA-CSIC*

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Flow and mixing at channel intersections are of broad interest because fluids with distinctive properties can efficiently mix and react at intersections, thereby controlling mixing and reaction processes in natural and engineered fractured and porous media. Recent studies showed that mixing and reaction hot spots are strongly linked with flow topological properties that form the backbone of underlying flow fields. In particular, stagnation points are related to strong stretching, folding, and flow separation, thereby governing overall mixing and reaction dynamics. Lee and Kang 2020 [Physical Review Letters, 124(14)] namely observed that inertia effects can induce recirculating flows at channel intersections and showed that the recirculating flows associated with stagnation points initiate local reaction hot spots, that is, locations where reaction rates are locally maximum. Nevertheless, there has been no systematic study on how diverse flow topologies emerge at channel intersections and how they control mixing and reaction dynamics at intersections.

In this study, we combine laboratory microfluidic experiments, pore-scale numerical simulations, flow topology analysis, and lamella mixing theory to establish a predictive framework that links flow

topological properties to mixing and reaction properties. We systematically vary both the injection rate and injection rate ratio between the two inlets to elucidate how various flow topologies emerge at channel intersections as a function of the Reynolds number and injection rate ratio. We then establish a quantitative link between flow topology, mixing, and reaction rates. Finally, we upscale mixing and reaction at channel intersections using the lamella mixing theory and show how the key parameters of the upscaled model can be estimated from the flow properties.

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Lee, S.H. and Kang, P.K., 2020. Three-dimensional vortex-induced reaction hot spots at flow intersections. *Physical review letters*, 124(14), p.144501. **Acceptance of Terms and Conditions:**

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MS20 / 142

## Upscaling between an agent-based model (smoothed particle approach) and a continuum-based model for wound contractions

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Deep tissue injury often results in contraction of skin due to mechanical pulling forces exerted by skin cells (fibroblasts) in the dermal layer. If contractions are morbid, then they are referred to as contractures. Contractures cause disabilities to patients, by, for instance, loss of mobility of a joint. By the use of modeling, we aim at understanding the mechanisms behind the formation of a contracture and at predicting which wound is likely to develop a contracture and which treatments can be employed in order to minimize the likelihood of a contracture. In most of our work, we used the immersed boundary approach based on a superposition of Dirac Delta functions to describe the forces exerted by individual skin cells, which results in a finite element solution that is not in H1. In [1, 2], we developed the smoothed particle approach as a replacement of the immersed boundary approach to improve the accuracy of the solution.

The smoothed particle approach is categorized as agent-based model, in which cells are considered as individuals. This class of models has the advantage of investigating the cellular activities of every single cell. Furthermore, for this modelling class, it is more straightforward to deduce parameter values from in vitro or in vivo experiments. However, once the number of cells is in the order of thousands and the wound scale is large (like centimeter square), these models become too expensive from a computational perspective. For the larger scales, continuum-based models are used. These models do not treat cells as separate entities, but treat cell behavior by the use of cell densities, which represent numbers of cells per unit volume. The resulting partial differential equations are easier to solve in terms of computational power.

We investigated the connections and consistency between these two types of models, regarding the momentum balance equation, which is used to describe the forces exerted by cells on the extracellular matrix (ECM) causing the deformation of the substrate. In one dimension, we establish the consistency between these approaches in both analytical solutions and finite-element method solutions. In the multi-dimensional case, we have only computationally shown the consistency between the continuum-based and agent-based models.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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## Upscaling of a Cahn–Hilliard Navier–Stokes Model including Precipitation in a Thin Strip

**Authors:** Lars von Wolff<sup>1</sup> ; Iuliu Sorin Pop<sup>2</sup>

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Multiphase flow and reactive transport are important in many applications, in particular in porous media. We consider the incompressible flow of two immiscible fluids in the presence of a solid phase changing due to precipitation and dissolution. We employ a ternary phase-field model on the pore scale, extending widespread models for two fluid phases by including a solid phase.

We upscale this model in the geometry of a thin strip. In the context of porous media the thin strip can be seen as the representation of a single pore throat. For scale separation we introduce  $\beta$  as the ratio between width and length of the strip. Using asymptotic expansions we investigate  $\beta \rightarrow 0$  under moderate assumptions on Peclet number and Capillary number. The resulting multi-scale model consists of upscaled equations for total flux and ion transport, while the phase field equation has to be solved in cell-problems on the pore scale to determine the position of interfaces.

We also investigate the sharp interface limit of the multi-scale model. Here the diffuse interface width  $\varepsilon$  approaches zero and a sharp interface model is recovered. The resulting model consists only of Darcy-scale equations, as the cell-problems can be solved explicitly. The model is of hyperbolic nature, and we use numerical results to investigate the validity of the upscaling when discontinuities form in the upscaled model.

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## Upscaling of two-phase flows in porous media

**Author:** Sohely Sharmin<sup>None</sup>

**Co-authors:** Iuliu Sorin Pop<sup>1</sup> ; Carina Bringedal

<sup>1</sup> *Hasselt University*



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We consider a mathematical model for two-phase immiscible flow in a porous medium. A solute is present in and transported by one fluid phase, leading to a non-constant surface tension. At the scale of pores, the main challenge is to account for the movement of the fluid-fluid interfaces, depending on the velocities and pressures of the two fluids, and on the concentration-dependent surface tension.

Using asymptotic methods, an upscaled, Darcy-scale model is derived. This is expressed in terms of effective macroscopic quantities, like saturation, concentration, pressure or Darcy velocity. In view of simplicity, we use first a two-dimensional strip as starting geometry at the pore scale. Then we consider a periodically perforated medium as a more general representation of a porous medium. In the former case, the evolving fluid-fluid interface is modelled as a freely moving sharp interface. In the latter case, a phase-field formulation is used. Employing asymptotic expansion methods and periodic homogenization, the corresponding Darcy-scale models are derived. For validating the results, we compare the numerical results for the Darcy scale models with those obtained by averaging the numerical results obtained for the pore-scale models.

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## Upscaling reactive flow and transport in evolving porous media

**Authors:** Nadja Ray<sup>1</sup> ; Stephan Gärttner<sup>2</sup> ; Peter Knabner<sup>3</sup> ; Peter Frolkovic<sup>4</sup>

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Porous media naturally exhibit a heterogeneous structure including two different spatial scales: The pore/micro-scale is the fundamental scale, on which flow and reactive transport processes take place whereas the macro-scale, i.e. the scale of the porous medium, is of practical relevance for geoscientific applications. What is more, mineral dissolution and precipitation alter a porous medium's structure and its bulk properties. Due to the medium's heterogeneity and lack in dynamic pore-scale measurements, there has been an increasing interest in effective models accessing such phenomena on the macro-scale without disregarding available micro-scale information.

In this talk, we start from a pore-scale model for reactive flow and transport in evolving porous media and derive an effective micro-macro model by formal two-scale asymptotic expansion in a level-set framework. As such, our approach comprises reactive flow and transport equations on the macroscopic scale including effective hydrodynamic parameters (porosity, reactive surface, diffusion, and permeability). These are calculated from representative unit cells. On the other hand, the macroscopic solutes' concentrations trigger mineral reactions, which alter the unit cells' geometrical structure.

Finally, we present numerical simulations of the fully coupled micro-macro problem with application to dissolution of calcite and dolomite.

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Poster + / 558

**Use of DNA tracers for determining aquifer hydraulic properties in a 3-dimensional laboratory sand tank****Author:** Swagatam Chakraborty<sup>1</sup>**Co-authors:** Rayan Elhaj<sup>2</sup> ; Chamath Akalanka Pamunugama Arachchilage<sup>3</sup> ; Jan Willem Foppen<sup>4</sup> ; Thom Bogaard<sup>5</sup> ; Jack Schijven<sup>6</sup><sup>1</sup> *Utrecht University, the Netherlands*<sup>2</sup> *IHE-Delft, Institute for Water Education*<sup>3</sup> *IHE-Delft, Institute for Water Education*<sup>4</sup> *Faculty of Civil Engineering and Geosciences, TU Delft; IHE-Delft, Institute of Water Education*<sup>5</sup> *Faculty of Civil Engineering and Geosciences, TU Delft*<sup>6</sup> *Department of Statistics, Informatics and Modeling, National Institute of Public Health and the Environment, Bilthoven; Chair, Quantitative Microbial Water Safety, Environmental Hydrogeology Group, Department of Earth Sciences, Utrecht University, Utrecht***Corresponding Authors:** j.foppen@un-ihe.org, s.chakraborty@uu.nl, rel002@un-ihe.org, cpa005@un-ihe.org, t.a.bogaard@tudelft.nl, j.f.schijven@uu.nl

DNA tracers have been applied in groundwater systems in order to track flow paths and travel times, and to identify hydraulic connections. In this study, we aim to develop a blueprint of the application of DNA tracers to determine hydraulic conductivity, effective porosity, and dispersion. Also, we aim to minimize the uncertainty in estimating the parameters. Two well-controlled laboratory built, ~130 x 70 x 40 cm and ~100 x 58 x 30 cm, respectively, Aquifer tanks were used under steady-state flow conditions. Under forced gradient condition, monodispersed, silica-coated double-stranded DNA tracer particles were injected and collected down-gradient. Different injection and sampling experiments were carried out: various well configurations, sampling depths, injection intervals and so forth. Water samples collected were analyzed on their DNA tracer concentration using a qPCR machine. Finally, the resulting breakthrough curves were analyzed to arrive at hydraulic properties, using groundwater flow and contaminant transport modeling (MT3DMS).

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**Use of infrared nano-spectroscopy to study the existence and thickness of the wetting film in oil-wet carbonates**

**Authors:** Tannaz Pak<sup>1</sup> ; Isadora Ferreira Caixeta<sup>2</sup> ; Luiz Fernando de Lima Luz Junior<sup>3</sup> ; Nathaly Lopes Archilha<sup>4</sup> ; Ingrid David Barcelos<sup>None</sup>

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In recovery of hydrocarbons from the subsurface wettability plays a key role. Wettability is a property controlled by the crude oil-brine-rock (COBR) interactions. It is known that wetting properties of a rock contributes to the microscopic oil displacement efficiency and the ultimate achievable recovery factor. Rocks (or rather minerals composing them) are water-wet at their initial (clean) state. It is commonly observed that long-term exposure of rock surfaces to heavy components of crude oil under high pressure and temperature conditions of subsurface hydrocarbon reservoirs causes the wetting to change towards more oil-wet. Heavy and polar organic compounds within crude oil (e.g. asphaltenes and resins) have the tendency to interact with the rock (mineral) surfaces resulting in adsorption of these compound onto the surface to form an oil film.

Understanding the scale of the oil film thickness as well as the main functional groups contributing to formation of these films are the underlying questions we address in this work. We present the outcome of a series of experiments using the infrared nano-spectroscopy beamline at the Brazilian synchrotron to study the COBR interaction at nano-scale. The IR1 beamline of the Brazilian synchrotron is equipped with a scattering Near-Field Optical Microscope (s-SNOM). Using this facility broadband infrared (IR) imaging and atomic force microscopy (AFM) topography can be performed with a lateral resolution of approximately 25 nm. It enabled us to perform an investigation on the surface of rock grains at clean and aged conditions.

The experiment was designed to investigate the interactions of a carbonate rock (Ketton limestone from England) with a crude oil (from Brazil) in presence of a brine (containing divalent ions). The crude oil was known to have significant levels of heavy components (e.g. asphaltenes and resins). Prior to the synchrotron session we prepared the samples by exposing several grains of this limestone to the crude oil following the aging procedure explained in Pak (2015)<sup>1</sup>. After the aging process the grains were sliced using an ultra-cryo microtome device to prepare ultrathin slices for use at the IR1 beamline. We focused on identifying the functional groups adsorbed to the grain surface by measuring line IR profiles starting from inside of a grain (where the IR signal detected pure calcium carbonate) moving towards the grain surface where the adsorbed organic compounds were expected. The measurements were repeated many times to overcome issues faced as a result of contamination of the cantilever tip which occurred as the tip approached the grain interface. We will also discuss the challenges we faced in cutting the samples and the impacts this has had on the observed signals. The infrared spectrum of absorption of the crude oil used in this study was recorded using a bench-top Fourier-transform infrared spectroscopy (FTIR) equipment. This spectrum is considered as the background IR signature of this crude oil as a whole. Collecting the broadband point spectra at different locations near the grain surface of the ultrathin sections reveals the chemical composition of the grain surface and the compounds adsorbed to it.

#### Time Block Preference:

Time Block A (09:00-12:00 CET) **References:**

Pak, T. Saturation tracking and identification of residual oil saturation. (The University of Edinburgh, 2015). **Acceptance of Terms and Conditions:**

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## Use of porous algal biochar in water treatment in the state of Ceará in Brazil

**Author:** Andre Frota<sup>1</sup>

**Co-authors:** Jose Capelo Neto<sup>1</sup> ; Erdin Ibraim<sup>2</sup> ; Tannaz Pak<sup>3</sup>

<sup>1</sup> *Federal University of Ceara*

<sup>2</sup> *University of Bristol*

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Growing world population and global warming impact the quality of water resources on a global scale. Eutrophication, the process of enrichment of water by nutrients, is considered one of the most common causes of water quality impairment. A direct outcome of eutrophication is an increase in the production of algae. In northeastern Brazil, a semi-arid climate region, cyanobacteria dominance and algae blooms are quite recurrent due to several factors, namely, high temperature, long photoperiods, and abundant nutrient availability. Water shortage and poor water quality are linked because contamination reduces the supply of water and increases the costs of treating water for use. Therefore, this poses a serious problem for a region with water scarcity and drought such as Ceará. In addition to the general deteriorating impact on the ecosystem, algae are associated with cyanobacteria which are known to produce toxic and/or noxious secondary metabolites that can render large quantities of water unsuitable for drinking. Cyanotoxins are primarily produced intracellularly and their release into the water makes the treatment process more costly, as well may pose a serious health hazard to animals and humans. Conventional methods of remediating persistent pollutants (agrochemicals, antibiotics, PAHs, PCBs, aromatic dyes, heavy metals, ammonia, nitrate, phosphate, sulfide, etc.) mainly employ methods that are costly and often generate large amounts of chemical residues (chemical precipitation, ion exchange, adsorption using activated carbon, and membrane separation processes), which have no economic value.

Biochar, a charcoal material, is an emerging material that has proven effective in environmental remediation and water treatment technologies. Biochar is produced using the thermal process of pyrolysis in which biomass feedstock is heated in absence of oxygen. As a result, an organic rich porous solid material is produced that alongside its use for environmental remediation can play a role in carbon sequestration and contribute to achieving net zero targets by reducing the emission of carbon dioxide. While efforts in manufacturing biochar have increased in the last decade, there is still a need for advancing the manufacturing processes (optimising the pyrolysis process) to improve biochar quality and quantity based on locally available feedstock. A key factor controlling the performance of biochar in environmental remediation applications is its multi-scale porous structure. To achieve a porous biochar an activation process (either chemical or physical) is required. In this study, we evaluate the use of drinking water treatment sludge as a feedstock for manufacturing porous biochar. We examine the possibility of applying the produced biochar to treat the contaminated water from which the algae were harvested. We use the algae from the Gavião water reservoir in the state of Ceará in Brazil.

The application of algal-biochar in water reservoirs in the state of Ceará will gradually control the occurrence of algae blooms. In the meantime, the use of algal-biochar in water treatment can contribute to creating a circular economy where the unwanted residue will be regarded as a feedstock for the production of biochar as a high-value product.

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Time Block C (18:00-21:00 CET) **References:**

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## Use of topological principles to determine wettability from pore-scale images

**Author:** Luke Kearney<sup>1</sup>

**Co-author:** Martin Blunt<sup>2</sup>

<sup>1</sup> *University of Oxford*

<sup>2</sup> *Imperial College London*

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There are numerous challenges associated with measuring the wettability of a porous material. Surface roughness and chemical heterogeneity obscure representative characterisations via contact angle hysteresis. Micron-resolution X-ray CT imaging has enabled direct geometric measurements of contact angle inside core samples but due to uncertainty and error at the contact line, this method tends to skew values towards 90°. The recent inception of an alternative topological approach has resulted in an approximate relationship between contact angle and interfacial curvature for individual clusters of the non-wetting phase, though its application has been limited to images of water-wet rocks at residual oil saturation. Here, previously published topological methods are demonstrated to be only applicable at these conditions. Furthermore, the wetting phase is not specified, leading to ambiguity for heterogeneous mixed-wet samples. We present a more generalised model to include any wettability and saturations with high phase connectivity. A practical workflow has been developed for application to experimental pore-scale images, with processing parameters optimised using results from lattice Boltzmann simulations. Correcting for the relative orientation of the contact line with the solid surface, lacking from previous methods, is shown to significantly reduce error. Comparison of measurements from both techniques on experimental and simulated images at similar conditions suggests that the topological approach presented here provides the more accurate quantification of contact angle for both water-wet and mixed-wet Bentheimer sandstone samples. Consistent 3D spatial distributions of contact angle for these images can now be observed, enabling wettability in porous media to be studied in much greater detail.

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## Using PIV and 3D printing to investigate fluid flow and solute transport in fractured porous media.

**Author:** Isamu Naets<sup>1</sup>

**Co-authors:** Mehrdad Ahkami ; Po-Wei Huang<sup>1</sup> ; Martin Saar<sup>1</sup> ; Xiangzhao Kong<sup>1</sup>

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Preferential flow-paths are well-known features in fractured rock masses, often allowing rapid movement of fluid and early breakthrough of solutes and/or heat/cold in a small fraction of void space, compared to non-fracture-dominated porous media. These preferential flow-paths can change as the configuration of fractures varies, due to, for example, shear displacement (Yeo et al.,1998; Kluge et al.,2017) or bifurcations (Li,2002; Johnson et al.2006). Such changes could become particularly important for subsurface projects, such as geothermal energy utilization, reservoir enhancement, and hydrometallurgy. Although numerical studies have shed some light on the preferential flow path and

fluid behavior in rough fractures, experimental visualization and, more importantly, quantification of flow paths in rough-walled fractures still remains a challenge.

In this work, we show how to record and quantify fluid velocities and solute transport rates through a rough fracture using Particle Imaging Velocimetry (PIV) measurements, which have been rarely applied in the geosciences (S.H. Lee et al., 2015; Ahkami et al., 2018). During PIV measurements, a solution of mineral oil and trans-anethole is prepared to match the refractive index of the clear 3D-printed fractures. This solution serves as the working fluid, seeded with nearly neutrally-buoyant fluorescent particles. In the first study, the PIV results on a single, rough, shear-able fracture will be compared to numerical simulations using the local cubic law. In the second study, we visualize solute transport and fluid flow through a bifurcating rough-walled fracture, quantified by PIV measurements and lattice-Boltzmann simulations.

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS6-A / 286

## Using colloidal deposition to mobilize immiscible fluids from porous media

**Authors:** Joanna Schneider<sup>1</sup> ; Rodney Priestley<sup>1</sup> ; Sujit Datta<sup>1</sup>

<sup>1</sup> *Princeton University*

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Colloidal particles hold promise for mobilizing and removing trapped immiscible fluids from porous media, with implications for key energy and water applications. Most studies focus on accomplishing this goal using particles that can localize at the immiscible fluid interface. Therefore, researchers typically seek to optimize the surface activity of particles, as well as their ability to freely move through a pore space with minimal deposition onto the surrounding solid matrix. Here, we demonstrate that deposition can, surprisingly, *promote* mobilization of a trapped fluid from a porous medium without requiring any surface activity. Using confocal microscopy, we directly visualize both colloidal particles and trapped immiscible fluid within a transparent, three-dimensional porous medium. We find that as nonsurface active particles deposit on the solid matrix, increasing amounts of trapped fluid become mobilized. We unravel the underlying physics by analyzing the extent of deposition, as well as the geometry of trapped fluid droplets, at the pore scale: deposition increases the viscous stresses on trapped droplets, overcoming the influence of capillarity that keeps them trapped. Given an initial distribution of trapped fluid, this analysis enables us to predict the extent of fluid mobilized through colloidal deposition. Taken together, our work reveals a new way by which colloids can be harnessed to mobilize trapped fluid from a porous medium.

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MS9 / 458

## Validation and calibration of interface conditions for Stokes-Darcy problems

**Author:** Iryna Rybak<sup>1</sup>

**Co-authors:** Elissa Eggenweiler<sup>1</sup>; Paula Strohbeck<sup>1</sup>

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Coupled free-flow and porous-medium systems described by the Stokes-Darcy equations are intensively studied in the last decade. Most of the coupling concepts are based on the Beavers-Joseph interface condition, which is developed for one-dimensional flows parallel to the fluid-porous interface. However, this condition is unsuitable for arbitrary flow directions [2], e.g. for industrial filtration problems. Alternative coupling concepts existing in the literature, e.g. 1 contain unknown coefficients, which need to be calibrated before they can be used in computational models. Pore-scale simulations play here an important role, both for the validation of the coupled macroscale models and for the computation and calibration of the effective model parameters.

In this talk, we present a comparison study of several coupling concepts for the Stokes-Darcy problem [3, 4]. Coupled macroscale models are validated numerically by comparison of the macroscale simulation results against the pore-scale resolved models. Effective parameters appearing in the alternative interface conditions [3] are computed numerically based on the geometrical configuration of the underlying problem. The exact location of the sharp fluid-porous interface and the Beavers-Joseph parameter in the classical conditions are optimized for different pore geometries. We show that the coupling conditions proposed in [3] are the most accurate ones and the Beavers-Joseph parameter cannot be fitted for arbitrary flows to the fluid-porous interface.

**Time Block Preference:**

Time Block B (14:00-17:00 CET) **References:**

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[2] E. Eggenweiler and I. Rybak: Unsuitability of the Beavers-Joseph interface condition for filtration problems. *J. Fluid Mech.*, 892, A10, 2020.

[3] E. Eggenweiler and I. Rybak: Effective coupling conditions for arbitrary flows in Stokes-Darcy systems. *SIAM Multiscale Model. Simul.* (in press), 2021.

[4] I. Rybak, C. Schwarzmeier, E. Eggenweiler, and U. Rde: Validation and calibration of coupled porous-medium and free-flow problems using pore-scale resolved models. *Comput. Geosci.*, 2020, doi:10.1007/s10596-020-09994-x **Acceptance of Terms and Conditions:**

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## Variations in Airflow Field and Soil Grain-Size of Simulated Shrubs with Different Spatial Configurations based on Wind Tunnel Experiments

**Authors:** Xia Pan<sup>1</sup> ; Zhenyi Wang<sup>1</sup>

<sup>1</sup> Inner Mongolia Agricultural University

**Corresponding Authors:** 18248113866@qq.com, panxia2019@gmail.com

Wind erosion is an ecological and environmental issue of global concern, with many adverse effects such as damage to infrastructure, economic loss, increased regional poverty, and social instability [1, 2]. Desertification directly caused by wind erosion affects 32% of the world's population, 67% of countries, and 40% of the land area, making it a serious threat [3]. The United Nations Convention to Combat Desertification (UNCCD) calls for attention and action to be taken in the science of combating desertification [4]. Extensive research has shown that that natural vegetative and artificial windbreak forests are the most widely used measure to reduce wind velocity and trap sand [5]. However, the construction of natural vegetative in arid and semiarid areas is limited by scarce water resources and unique soil texture [6]. On the contrary, artificial windbreak forests have been successfully applied in wind and sand engineering projects with low cost and water demand that effectively reduce wind speed and trap sand particles. Although windbreak forests have been implemented to control wind erosion for many years as a wind erosion control measure in arid and semiarid areas, there are few studies on the comprehensive efficiencies between the geometric configuration and spatial arrangement of windbreak forests in terms of the near-surface airflow field and soil grain-size variation, and there are still controversies regarding the optimal design of windbreak forests to maximize the efficiency of the windbreak forests. Given this, we designed a series of wind tunnel experiments with the first goal of clarifying the variations of the near-surface airflow field and soil grain-size of simulated shrubs (equivalent to windbreak forests) with different spatial configurations that contain three form configurations (spindle-shaped, broom-shaped, and hemisphere-shaped) and row spaces (17.5×17.5 cm, 17.5×26.25 cm, and 17.5×35 cm) under the net wind speeds of 8 m/s, 12 m/s, and 16 m/s. Our object was to reveal how to arrange the windbreak forests in terms of form configurations and row spaces for preventing desertification in the most convenient and efficient ways. A better understanding of the airflow field and soil grain-size around the simulated shrubs is essential to provide optimized design and maximize the efficiency of the windbreak forests. Simulated shrubs used in this study are not only polymerized by anti-aging polymer compounds which are new wind-resistant materials but also it has beautiful visual effects in deserts.

### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

1. Shen W, Li H, Sun M, Jiang J. Dynamics of aeolian sandy land in the Yarlung Zangbo River basin of Tibet, China from 1975 to 2008. *Global and Planetary Change*. 2012, 86: 37-44.
2. Chen X, Duan Z, Tan M. Restoration Affect Soil Organic Carbon and Nutrients in Different Particle-size Fractions. *Land Degradation & Development*. 2016, 27: 561-572.
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## Viscous Fingering in Miscible Displacements in Porous Media with Dead-End Pores

**Authors:** Baizheng An<sup>1</sup> ; Qingwang Yuan<sup>1</sup>

<sup>1</sup> *Texas Tech University*

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The finger-like instabilities, referred to viscous fingering (VF), are commonly observed when a less viscous fluid displaces a more viscous fluid in a Hele-Shaw cell (two parallel plates with a small gap) and porous media. It is well recognized that the VF can reduce the sweep efficiency of displacement processes. But in the SWEPT area by injected fluids, the existing numerical modeling shows that nearly no displaced fluid is left. This is valid for the fluid flow displacements in porous media with all well-connected pores. However, real porous media, such as subsurface rocks, especially the carbonate rocks, have non-negligible proportion of dead-end pores, the stagnant volume in which fluid is nearly immobile and cannot be directly displaced. The only mechanism for mass transfer from dead-end pores to well-connected pores is diffusion or dissolution. The consequence is that such trapped fluids cannot be cleaned up by injected fluids. Accordingly, the swept area behind the VF still has a certain amount of displaced fluids, depending on the mass transfer rate and proportion of dead-end pores.

To investigate the VF dynamics in porous media with dead-end pores, we assume the miscible displacements take place in a two-dimensional horizontal porous medium with a uniform distribution of dead-end pores. We conducted numerical simulations to model the displacement processes. We found that the VF dynamics is strongly affected by the dead-end pores. Specifically, the proportion of dead-end pores and dissolution rate from fluids from dead-end pores to well-connected pores play an important role. The larger proportion of dead-end pores leads to earlier breakthrough of the injected fluids but more residual displaced fluids. However, the influences of dissolution rate on VF are non-monotonic. There is a range of dissolution rate that lead to the least unstable VF in miscible displacements. The dissolution fingering in the dead-end pore network is reported for the first time.

This research has wide applications in a series of displacement process involving porous media such as soil and water contaminate remediation, CO<sub>2</sub> sequestration, enhanced oil recovery, geothermal recovery, drug delivery, and chromatographic separation.

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## Visualization Research of Clay Mineral Migration in Low Salinity Water Flooding Based on 2.5D Microfluidic Model

**Author:** Fei Xu<sup>1</sup>

**Co-authors:** Hanqiao Jiang<sup>1</sup> ; Shiyuan Qu<sup>1</sup> ; Fuwei Yu<sup>1</sup> ; Junjian Li<sup>1</sup>

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**Objectives/Scope:** There have been many reports on EOR by low salinity water flooding. An inevitable phenomenon of low salinity water flooding is that clay minerals would undergo hydration

expansion and be washed off from the rock, and then migrate in the pore throat. In this study, a 2.5D visualized microfluidic model is used to observe and analyze various phenomena during the migration of clay minerals, including blockage in the throats and adsorption of clay minerals on the surface of crude oil, as well as their effects on oil recovery.

**Methods, Procedures, Process:** A 2.5D microfluidic model is prepared that has a homogeneous porous structure with micro-sized pore throats. A mixture of chlorite and low salinity water would be injected into the model to simulate the migration of clay minerals. And three groups of experiments are designed, including the clay mineral migration experiment with or without crude oil being pre-saturated, and the control experiment of low salinity water drive crude oil without clay mineral. Then the phenomena of clay mineral migration would be visualized under the microscope.

**Results and Observations:** We have observed the phenomenon that clay minerals gradually accumulate at the throat and block the throat. And we also found that when the injection speed is low, the clay minerals could migrate to the throat far away from the entrance and block the throat. After the speed is significantly increased, clay minerals would tend to accumulate and block the throat at the entrance. This phenomenon indicates that the displacement speed of low-salinity water flooding should not be too high. We have also observed the phenomenon that clay minerals were adsorbed on the surface of oil droplets. The occurrence of this phenomenon would increase the migration resistance of oil droplets, which is not conducive to the exploitation of crude oil. In addition, we have also observed the phenomenon that the water phase diffused into the oil phase under low salinity water flooding. This phenomenon has been reported in many papers as one of the important oil displacement mechanisms of low salinity water flooding.

**Novel/Additive Information:** The migration of clay minerals is a common phenomenon in low-salinity water flooding. However, there are few visual studies on the migration of clay minerals. Based on the 2.5D visualization microfluidic model, this study observed the phenomena that occurred during the migration of clay minerals and analyzed their influence on oil recovery, which would be helpful to improve the understanding of the role of clay minerals migration.

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MS3 / 357

## Visualization and segmentation of micro-cracks based on X-ray computed tomography imaging

**Authors:** Dongwon Lee<sup>1</sup> ; Matthias Ruf<sup>2</sup>

**Co-authors:** Nikolaos Karadimitriou<sup>3</sup> ; Holger Steeb<sup>4</sup>

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The thermal treatment of rocks is a frequently used method to initiate micro-cracks. This is done to study experimentally different physical phenomena related to micro-cracks. The effect of micro-cracks on the effective macroscopic properties can be quantified, for instance, by wave propagation measurements or porosity measurements. Micro X-Ray Computed Tomography ( $\mu$ XRCT), as a non-invasive imaging method, offers the possibility to have an insight into the 3D microstructure. With

this method, it is possible to improve the understanding of the relation between the micro-scale and the effective properties. Since micro-cracks have a disadvantageous ratio between the crack aperture and the crack length, the imaging, as well as the subsequent segmentation, is a challenging task. In particular, the spatial resolution of  $\mu$ XRCT devices often come to its limitation to resolve the crack aperture reliable. Furthermore, an inherent noise and low contrast of the resulting dataset cause difficulties to achieve an accurate segmentation. Based on an in-house created  $\mu$ XRCT data set of a thermally treated Carrara marble sample, we applied and compared different segmentation methods. By all methods, the full 3D crack network can be successfully segmented. However, an approach based on a 2D Convolutional Neural Network (CNN) model shows the most promising result among the adopted methods. The segmented data is frequently used as direct input, for instance, in digital rock physics. Consequently, all the results depend on the quality of the imaging and the segmentation. Therefore, it is crucial to evaluate the quality of the segmentation. For this, a link back to macroscopic measurement results, for instance, the porosity can be used as an indicator. Besides different segmentation approaches, this contribution shows the importance of combining measurements of different scales, especially to evaluate segmentation methods.

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## Visualization of optically opaque flow systems through lab-based, dynamic X-ray micro-CT

**Author:** Jan Dewanckele<sup>1</sup>

**Co-authors:** Marijn Boone<sup>1</sup> ; Luke Hunter<sup>2</sup> ; Andreas Griesser<sup>3</sup> ; Christian Wagner<sup>4</sup> ; Simo A. Mäkiharju<sup>5</sup>

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Single and multi-phase flow are encountered almost everywhere, including biological and chemical processing, offshore applications, oil and gas recovery, corrosion and naval hydrodynamics. Extending the physical understanding of single and multi-phase flow is of key importance of many industrial applications. High-speed visualization, such as particle image velocimetry (PIV) has been successfully applied to capture flow processes in detail for many of these flows. However, for some set-ups, light might scatter between vapor and liquid phases or more severely, be completely blocked.

In Previous work, to overcome this limitation of PIV, a medical X-ray source coupled with a high-speed imager was used to study the void fractions in ventilated and cavitating flows (Mäkiharju et al., 2013). The system was capable of acquiring two-dimensional projections through an O(10 cm) water column at rate of 1kHz with spatial resolution below 1 mm. In general, when using experimental techniques to study the behavior of flow, they ideally should have both a high spatial and temporal resolution to resolve the dynamics of the flows. Because of their high fluxes, synchrotron facilities are well suited to perform those dynamic experiments (Duke et al., 2015). Imaging of dynamic processes is one of the key applications at synchrotron facilities, pushing the time resolution

more and more down with quite some success. However, access to those facilities is often limited and operational cost are quite high.

The flows of industrial interest typically require imaging rates much higher than achievable with conventional micro-CT laboratory systems. If the acquisition time is slower than the flow speed relative to the resolution, temporally induced blurring is induced. However, recent developments at TESCAN XRE have made it possible to image, reconstruct, and inspect dynamic processes in the laboratory with a temporal resolution of a few seconds. These developments are not only enabling investigation of low Reynolds number opaque flows in great detail, but also clogging processes in porous media. For the latter, for example mobilization and clogging of clay can significantly change the transport properties in porous rock materials. Segmentation and analysis of the seeding particles was performed by using the Software GeoDict.

In this study, we demonstrate the capabilities of visualizing flows in 3D in optically opaque containers or materials by using in-lab X-ray micro-CT. The proof-of-concept experiments resulted in the visualization and analysis of particles in creeping flows. Silver coated hollow particles were used as flow tracers in a liquid (water-glycerol mixture). Hundred full rotations were acquired with a total scan time per rotation (0-360°) of 2.9 seconds. This resulted in both the visualization and analysis of the flow behaviour in opaque systems.

#### ACKNOWLEDGEMENTS

The last author gratefully acknowledges the support of NSF EAGER award #1922877 program manager Ron Joslin and Shahab Shojaei-Zadeh.

#### Time Block Preference:

Time Block B (14:00-17:00 CET) **References:**

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MS16 / 197

## Visualizing imbibition in thin porous media with high-speed NMR

**Authors:** Ruben Nicasy<sup>1</sup>; Henk Huinink<sup>1</sup>; Bart Erich<sup>1</sup>; olaf adan<sup>2</sup>

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The imbibition of liquids in thin, porous films is a widely studied phenomenon [1]. For example, in the print industry, understanding the penetration of ink inside paper provides tools for improving the quality of the print. However, measuring inside submillimeter opaque films like paper with a high temporal resolution is a challenging task. Here we introduce a Garfield Nuclear Magnetic resonance [2] (NMR) approach for measuring liquid imbibition into thin, porous films. Firstly, we were able to measure liquid distribution inside porous films with a spatial resolution of 100 μm on a time scale below 0.1s. Moisture profiles were measured for different model liquids inside PVDF and cellulose nitrate membranes. Secondly, microliter sized droplets were used to study the penetration process inside thin porous PVDF membranes (approx. 110 μm). Moisture profiles were measured with time frames as low as 25ms, which is to our knowledge the fastest NMR measurement used to study penetration ever reported. The front position inside the membranes, is determined from

the liquid profiles, which allows to quantify the imbibition process. To illustrate the experimental power, the effect of viscosity and pore radius on the penetration process were investigated. To study the effect of pore size, two different PVDF membranes with a well-defined pore radius of 0.65 and 0.22  $\mu\text{m}$  were tested. The penetration process was performed with different water-glycerol mixtures to study the effect of viscosity on the process. First results show a rather sharp imbibition front, additionally the imbibition dynamics obeys Stokes' flow, but cannot be explained with the classical Lucas-Washburn equation [3]. The presented high-speed NMR imaging approach allows to measure the motion of liquid fronts on time and length scales that were not accessible before.

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## Water infiltration to sandstone outcrops at the soil-rock interface

**Authors:** Martin Slavík<sup>1</sup> ; Tomáš Weiss<sup>1</sup> ; Ondřej Sysel<sup>1</sup> ; Martin Lanzendorfer<sup>1</sup>

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Water acts as a very important agent in salt and frost weathering responsible for major physical damage to both natural rocks and building stones, and compared to the idealised laboratory research, distinctly fewer field studies investigated water's role in weathering processes on natural rock exposures. Especially, there is a lack of knowledge about the critical interaction between soil and rock as one of the types of water entrance into natural rock outcrops. In Český ráj (Czechia), we studied water flow dynamics at this soil-rock interface by measuring the infiltration rate into natural sandstone surfaces (Karsten tube) and water content (TDR) in a shallow zone (cca 0.8 m) of soil 1. The results show that, as the underlying sandstone is coarser than the soil cover, water infiltrates to the rock only when water content reaches a certain threshold (roughly 17–27 vol. %), and at lower saturations the soil cover retains all the rainwater. The most notable finding is that the infiltration rate (m/s) of the sandstone surfaces differed up to four orders of magnitude over a distance of tens of meters, mostly depending on the weathering degree of the surface. The hydraulic properties of natural rock outcrops in weathering/water flow studies should therefore be interpreted with extreme caution as these are likely to significantly differ within a study area. Our results also show that to quantify the entry of water into sandstone outcrops, one should consider not only the permeability of the surface, but also other factors such as the presence and hydraulic properties of the soil cover which can function as a water reservoir enabling rock-infiltration of otherwise run-off rainwater. A less time and resource demanding methodology to investigate hydraulic parameters of both soil and the underlying rock would be beneficial. In a follow-up study, we intend to investigate a method using non-Newtonian fluids such as xanthan solution to measure hydraulic conductivity and pore size distribution of both the soil and the underlying rock. Similar approach using a set of saturated flow experiments has been already successfully applied [2, 3], where the authors described pore size distribution of various porous media.

This research is funded by the Czech Science Foundation [GA21-27291S].

**Time Block Preference:**

Time Block A (09:00-12:00 CET) **References:**

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MS13 / 320

## Water transport in soft nanoporous materials: Impact of mechanical deformation on collective dynamics, interfacial slippage and permeance

**Authors:** Alexander Schlaich<sup>1</sup> ; Matthieu Vandamme<sup>2</sup> ; Marie Plazenet<sup>3</sup> ; Benoit Coasne<sup>4</sup>

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Transport of water in soft porous materials is relevant to a broad range of applications such as ultrafiltration and reverse osmosis processes, where polymeric membranes are employed in filtration/separation, or energy related processes where proton conducting media (Nafion for instance) are used. It also pertains to important fields such as those dealing with wood/cellulosic materials, food processing and is of utmost importance in many biological processes (transport through cellular membranes). While water transport in hard porous materials such as porous silica glasses is well studied, the situation in soft matter is much more puzzling and remains unclear due to the combination of surface heterogeneity, the diffuse boundary location and pore deformations due to mechanical stresses.

In this work we study water in chemically realistic hydrophobic pores at different thermodynamic and mechanical conditions using atomistic molecular dynamics simulations. In detail, we show that the pore swelling can be modeled within a poromechanic framework and analyze the adsorption and confinement effects as well as microscopic diffusion mechanisms and transport effects due to pore size fluctuations. Strikingly, we found that hydrodynamic continuum models remain valid for planar flow of water even in monolayer confinement in soft pores.

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## Wettability behavior of preserved core material compared to dry stored core plugs during a low salinity water core-flooding investigation

**Author:** Rasoul Mokhtari<sup>1</sup>

**Co-authors:** Armin Afrough<sup>1</sup>; Karen Feilberg<sup>1</sup>

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Low salinity water-flooding is an EOR method that potentially modifies the equilibrium of the crude oil/brine/rock (COBR) system to a condition that allows additional oil to be mobilized in the porous media. The uncertainties associated with this EOR method, which has been demonstrated extensively in sandstones and some carbonates, are greater when dealing with a realistic crude oil containing polar components and a rock with highly reactive surfaces. Amongst carbonates, chalk reservoirs are particularly challenging due to their low matrix permeability, high porosity, high degree of heterogeneity, and a high tendency for surface reactions with both crude oil and brine. In the literature, experiments on outcrop chalk cores have been extensively reported, however, there is still a lack of data for reservoir chalk material, and further, there are no results on preserved core material showing how differently they might behave compared to dry stored reservoir core plugs. Preserved core plugs have been stored in a sealed condition with the fluid retained inside the core, while dry stored core plugs have been left open to drying and evaporation of all but the heaviest oil components. There is thus a question of how the wetting condition of the reservoir is represented by the two types of samples. Therefore, besides investigating the role of brine salinity on oil recovery, this work aims to evaluate the effect of using preserved core material on the results through a series of systematic core-flooding experiments on cleaned and dry stored cores and preserved reservoir material. For this purpose, using computed tomography results, reservoir chalk core samples (dry and preserved) without any open fractures were selected. These cores were saturated with reservoir fluids and aged at reservoir conditions for three weeks. Several synthetic brines were introduced through different injection scenarios into the aged cores at reservoir conditions. Insights into the role of brine chemistry were obtained through effluent analyses performed using ion chromatography. Furthermore, the COBR interactions were investigated through post-flooding NMR relaxation time measurements.

Results showed that diluted seawater, compared to normal seawater, has a significant effect on oil recovery when injected at the secondary stage. It is worth mentioning that formation water showed almost the same recovery potential as diluted seawater. Calcite dissolution, deposition of a magnesium-containing phase and the release of sulfate ion were observed at these experimental conditions during DSW injection, even though brines were equilibrated with calcite at room temperature. NMR relaxation experiments reveal that the rock surface for the preserved core is more oil-wet still after the first core flooding experiment, and changes to a more water-wet state after the second experiment on the same core. This means that although a preserved core sample may mimic the reservoir condition better, core flooding results on the same core may not be directly comparable.

Effluent brine analyses and NMR relaxation provide a large body of data that elucidate rock-brine-oil interactions during core-flooding. This work complements low-salinity recovery data in the literature that, at this point, is completely lacking in information from Danish chalk reservoirs.

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MS6-A / 620

## Wettability effects on multiphase displacements in heterogeneous porous media

**Authors:** Wenhai Lei<sup>None</sup> ; Moran Wang<sup>1</sup>

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We have studied wettability effects on multiphase displacements in heterogeneous porous media by experiments on microfluidic chips. The developed analysis method on high-resolution images enabled us to link pore-scale physics and macroscopic consequences. By varying fluid properties to achieve a wide range of contact angles  $\theta$  ( $23^\circ \leq \theta \leq 127^\circ$ ), we find a non-monotonic rule of wettability effects on displacement efficiency on the heterogeneous porous structure which leads to a consequent preferential flow, in contrast to a monotonic one of wettability effects on the homogeneous matrix structure. Similar to nature, for the flow on heterogeneous porous media, there is a critical wettability for the best displacement efficiency. Pore-scale mechanisms are identified to elucidate these behaviors: cooperative pore filling in the intermediate water-wet condition cause the maximum displacement efficiency; corner flow in strong water-wet condition and Haines events in strong oil-wet condition will decrease displacement efficiency. Our findings shed unique insights on how the interaction between wettability and preferential flow pathway affects fluid displacement in porous media.

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## **Wetting, Imbibition and Switchable Elastocapillarity in Nanoporous Media**

**Author:** Patrick Huber<sup>1</sup>

<sup>1</sup> *Hamburg University of Technology*

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Liquid-infused nanopores play a pivotal role in many natural and technological processes ranging from transport across biomembranes and plant movements to templating processes for nanomaterials and modern concepts of water desalination. Here I will present three experimental studies aimed at the fundamental exploration of wetting and imbibition dynamics in and at nanoporous surfaces (1) as well as studies aimed at employing the coupling of the elasticity of solids with the nano-capillarity of liquids, most prominently water, for the design of adaptive and electrically switchable actuator materials (2,3). To that end opto-fluidic techniques employing photonic crystals will be combined with cyclic voltammetry and high-resolution synchrotron-based X-ray analytics.

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## Investigation of water freezing in gas diffusion layer of PEMFC using lattice Boltzmann method

**Authors:** Gao Yuan<sup>None</sup> ; Jin Teng<sup>None</sup> ; Ding Zhaofeng<sup>None</sup>

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Lattice Boltzmann method, as a mesoscopic kinetic model between the macro-continuous model and the micro-molecular dynamics model, is a special discretization format, which is simple and efficient, and can solve the multiphase in complex geometric structures 1. The characteristics of multi-component flow are widely used in solid-liquid phase change simulation. The key feature of the solid-liquid phase change problem is that the phase interface separating the solid and liquid phases dynamically evolves over time. The main challenge in simulating this problem is that the location of the phase interface is coupled with the heat transfer process.

The gas diffusion layer of PEMFC is a typical porous structure, composed of a carbon base layer with a complex pore structure and a microporous layer. In order to ensure the normal operation of PEM, it is usually necessary to maintain a water balance inside the cells. In this paper, the lattice Boltzmann method based on total enthalpy is used to simulate the water freezing problem under the two-dimensional scale in the reconstructed model of carbon paper GDL by using double distribution functions of velocity field and temperature field. Dimensionless time and dimensionless temperature distribution is used to characterize the freezing process of water. For the boundary condition of the velocity field, the standard non-slip rebound format is uniformly adopted, and for the boundary condition of the temperature field, the non-equilibrium extrapolation format is adopted [2]. The initial state is set to be that the pore area is evenly filled with liquid water. The left wall of the simulation object adopts a constant temperature boundary condition, a constant external low temperature is suddenly applied to the left wall, and the other three walls adopt a completely insulated boundary condition, so a phase change heat conduction channel can be formed between the left and right walls. The pore area starts to freeze from the left end, and the phase interface is unevenly shaped due to the influence of different thermophysical parameters of the porous medium. With the passage of time, the phase interface gradually moves to the right and the moving speed gradually becomes slower. The reason is that the temperature gradient in the liquid phase region becomes smaller, causing the heat transfer process to slow down.

In addition, the natural convection phenomenon during the freezing process is also considered. In the solidification process dominated by heat conduction, due to the combined effects of volume changes, density differences of various parts and gravity, fluid flow and heat transfer will occur in the flow field. In the simulation, streamlines are used to characterize natural convection phenomenon. The density of streamlines represents the intensity and the arrow represents the direction of natural convection. Through simulation, it is found that there is a counterclockwise fluid flow in the liquid phase region that has not frozen, and there obvious vortex in the closed pore region formed by randomly distributed carbon fibers, which indicates that the shape of the solid-liquid interface mainly depends on the distribution of carbon fibers.

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MS9 / 587

**the impacts of pore-scale two-phase flow on mineral reaction rate****Author:** Hang Deng<sup>1</sup>**Co-authors:** Pei Li<sup>1</sup> ; Sergi Molins<sup>1</sup><sup>1</sup> *Lawrence Berkeley National Laboratory***Corresponding Authors:** hangdeng@lbl.gov, smolins@lbl.gov, lipei@lbl.gov

In various natural and engineered systems, multi-phase flow and mineral-fluid interactions co-occur and their interplay controls the evolution of these systems. In continuum scale models, how multi-phase flow dynamics affect mineral reactions are rarely accounted for or are corrected via reactive surface area and saturation of the aqueous phase. To evaluate the applicability of such treatment, understanding of the pore-scale dynamics is required. In this study, we developed a framework that couples the two-phase flow simulator from OpenFOAM with the geochemical reaction capability of CrunchTope, to examine pore-scale dynamics of two phase flow and their impacts on mineral reaction rates. For our investigations, flat 2D channels and single sine wave channels were used to represent smooth and rough geometry. Calcite dissolution in these channels were quantified with single phase flow and two phase flows with different saturations. We observed that the bulk calcite dissolution rates were not only affected by the loss of reactive surface area as it becomes occupied by the non-reactive non-aqueous phase, but also largely influenced by the changes in local velocity profiles due to the presence of then non-aqueous phase. The extent of the changes in reaction rates in the two-phase systems compared to the corresponding single phase system is dependent on the flow rate (i.e., capillary number) and channel geometry. The pore-scale simulation results can be used to better constrain reaction rate descriptions in multiphase continuum scale models.

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**‘Cocktail effects’ of co-existing hydrocarbon on heavy metal remediation****Authors:** Anuradha Garg<sup>1</sup> ; Brijesh Kumar Yadav<sup>1</sup>**Co-authors:** Shashi Ranjan<sup>1</sup> ; Amit Vatsa<sup>1</sup><sup>1</sup> *Indian Institute of Technology Roorkee***Corresponding Authors:** avamit179@gmail.com, shashishashi21@gmail.com, agarg@hy.iitr.ac.in, brijesh.yadav@hy.iitr.ac.in

Pollution of soil-water resources due to industrial, domestic and agricultural activities is a growing concern. The polluted soil-water systems contain a mixture of organics, heavy metals, hydrocarbon oils, emerging compounds etc. These ‘pollutant cocktails’ exhibit interesting interactions by altering chemical activity of individual pollutants in the system. Heavy metals and petroleum hydrocarbons are two commonly found soil-water pollutants. Surface adsorption using nano-zerovalent iron

(nZVI) is a popular remediation method for heavy metal removal in soil-water; however, its application in the presence of other contaminants is seldom studied. In the present study, we investigated the effect of co-existing petroleum hydrocarbon (toluene) on the removal of chromium using nZVI. The results represent the antagonizing effect of toluene on Cr (VI) removal and a reduced overall removal efficiency. The changing experimental conditions (pH and initial concentration) also showed significant effects on the removal efficiency. The efficiency was highest for lower pH conditions (pH = 3) and at lower initial Cr (VI) concentration (25 mg/L). The results, however, were different in the co-presence of toluene hydrocarbon. This study demonstrated important results for understanding the remediation challenges associated with mixed-contaminated soil-water systems.

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