InterPore2018 New Orleans

Monday 14 May 2018 - Thursday 17 May 2018

New Orleans

Report of Abstracts
This is an auto-updated version of the submitted contributions for InterPore2018 New Orleans
Parallel 1-B / 617

'Microbial Mortar' - restoration of degraded marble structures with microbially induced carbonate precipitation

James Minto¹; Rebecca Lunn¹; Grainne El Mountassir²; Qian Tan³; Hongxian Guo¹; Xiaohui Cheng¹

¹ University of Strathclyde
² University of Strathclyde, Glasgow, United Kingdom
³ 2Department of Civil Engineering, Tsinghua University, Beijing, China

Corresponding Author(s): rebecca.lunn@strath.ac.uk

Ancient stone relics and historic buildings are often subject to significant degradation. The protection and restoration of these monuments is extremely urgent. Here, a method of building repair based on microbial induced carbonate precipitation (MICP) has been tested on marble stone. In previous research, microbial mortar (stone powder treated by MICP) was tested as a filling material to repair cracks within stone. In this paper, the effect of microbial treatment on degraded marble consisting of larger particle sizes is studied. In the experiment, we focus on altering the permeability and porosity of crushed marble grains and show that the porosity and the permeability of the sample are notably decreased by carbonate precipitation.

MICP treatment is carried out in a column filled with marble grains with the injection of six batches over six days. A white CaCO₃ precipitate is produced which matches the original marble colour and is sufficiently strong to cement the marble sand together from the inlet up to a depth of 150 mm into the column. To understand the micro-scale distribution of the CaCO₃ precipitation within the column, and its effect on flow and transport properties, we analyse the MICP-treated column using X-ray CT with a resolution of around 3 microns. The X-ray CT scan data, support the macro-scale observations of a gradient in the degree of cementation along the direction of liquid flow, indicating that producing an evenly solidified sample is a problem that needs to be resolved.

We use the core-scale experimental data to derive cm-scale fluid transport properties using tracer breakthrough curves taken, prior to, and after MICP treatment. The fitted transport properties show that the fraction of pores containing mobile water decreases with increasing cycles of MICP. Pore-scale modelling using the X-ray CT data supports these findings, showing that cementation leads to a change in the pore network structure, with flow increasingly focussed into a smaller number of faster moving open channels.

Our experiments show that CaCO₃ precipitation is greatest at the inlet. It is reasoned that this could be avoided by modification to the injection strategy. Prevention of re-agent mixing outside the marble grains, careful choice of marble grain size distribution, and tailored injection flow rates could deliver re-agents deeper into the media and take advantage of the formation of stable flow pathways to maximise seal uniformity. MICP is a promising technique for the restoration of marble structures and monuments.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-D / 313

3D Imaging of flow pattern in natural porous media under low flow rate

Sabina Haber-Pohlmeier¹; Petrlik Galvosas²; Lutz Weihermüller³; Andreas Pohlmeier⁴

¹ ITMC, RWTH Aachen University
Understanding root water uptake is indispensable for the optimization of plant growth and crop yield against the background of growing world population. One strategy to understand how root water uptake functions is the knowledge of water flow from bulk soil to the root, passing the root-soil interface: the bottleneck for water uptake. Whereas direct flow imaging of fluxes in the above-ground plant stem has been performed by the group of Van As[1], little is known about flow pattern and velocities in the soil-root compartment. This is due to the low flow velocities based on the transpiration rate of the plant resulting in velocities of some tens of micrometer per second. Recently, it has been shown by Spindler et al. [2] that mean flow rates of a homogeneous flow as low as 0.06 mm/s can be measured even under the influence of internal magnetic field gradients using 13-interval stimulated echo multi-slice imaging (STEMSI).

In this work we extend the mapping of low flow velocities with STEMSI on heterogeneous flow patterns occurring by draining around a suction cup with a diameter of 5 mm set into fine sand. Time independent flow was regulated using constant external pressure difference to define the boundary conditions for later numerical simulation. The position of slices was chosen so that three different types of flow regimes were represented: At a sufficient distance above the suction cup homogeneous plug flow was monitored. Directly above the cup, flow converged to the center of, with the highest flow velocities in vertical direction in the center. The convergence became obvious by the x and y components of the flow velocity vectors which point unambiguously to the center. In the capillary below the suction cup we found the expected parabolic flow velocity profile. These experimental patterns have been reproduced satisfactorily by numerical simulations using 2D axissymetrically simulation using the Richards equation based Hydrus2D software[3]. These experiments have been extended to monitor flow pattern occurring in a real soil – plant system, and first results will be presented.

References:


Acceptance of Terms and Conditions:

Click here to agree

Poster 2 / 320

3D Reconstruction and permeability calculation from 2D thin sections

Yuqi Wu\textsuperscript{1} ; Chengyan Lin\textsuperscript{2} ; Lihua Ren\textsuperscript{2} ; Muhammad Jawad Munawar\textsuperscript{3} ; Yang Wang\textsuperscript{4}

\textsuperscript{1} China University of Petroleum (East China)  
\textsuperscript{2} China University of Petroleum (East China)  

Corresponding Author(s):
Permeability prediction of porous media is of great significance for both petroleum and environment fields. The permeability of a porous medium can be directly calculated based on one 2D thin section. However, it is often doubtful. Therefore, a new technique of the permeability prediction from a 2D thin section is proposed. First 3D porous media is reconstructed from a 2D image using multiple-point statistics. Then the single- and two-phase flow simulations are carried out based on the reconstructed 3D porous media. The absolute permeability is calculated by computing Navier-Stokes equation and Darcy’s law. The relative permeability is predicted using pore network method. In order to validate the method, the permeability calculation results are compared with them which are computed from the 3D real porous medium obtained using micro-CT scanner. The comparison shows that the technique is reliable, which offers petroleum and environment researchers a novel method for predicting the permeability when a 2D thin section is available.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-G / 331

3D simulation-based study of shear-thinning fluid flow in a sandstone fracture

Min Zhang1 ; Maša Prodanović1 ; Maryam Mirabolghasemi2

1 The University of Texas at Austin
2 Mississippi State University

Corresponding Author(s): minzhang@utexas.edu

Shear-thinning fluids flow in the rough fracture is encountered in numerous industrial applications such as hydraulic fracturing fluids flow in rough hydraulic and natural fractures to carry the propants, polymer gel extrusion through rough fracture to reduce excessive water production in naturally fractured reservoirs, CO2 sequestration and leakage through rough fractures, etc. We investigate both the macroscopic flow behavior and microscale flow details of shear-thinning fluids through a realistic rough fracture for both linear and inertial flow regimes.

For the first time, a fully-3D flow simulation of Cross power-law shear-thinning fluids through a rough fracture is conducted. The flow domain is extracted and refined from a computed microtomography image of a fractured Berea sandstone. The modified Navier-Stokes equation incorporating Cross power-law fluid rheology model is solved. The critical Reynolds number above which the linear Darcy’s law is no longer applicable is evaluated for both Newtonian and shear-thinning fluids.

First, the Newtonian fluid flow simulations are conducted, and the hydraulic/equivalent aperture and inertial coefficient in Forchheimer’s equation are fitted. Second, based on the simulation results of shear-thinning fluid flow, both the shift factor and inertial coefficient are obtained. Specifically, the shift factor is a critical parameter in the definition of “in-situ shear rate” which could be used to evaluate the “equivalent” viscosity based on the “bulk” viscosity. Our results show that the shift factor is dependent on both the fracture geometry and fluid rheology properties while both the inertial coefficient and critical Reynolds number are only functions of fracture geometry, which is consistent with the recent experimental results. Third, to explain the above phenomena, a detailed analysis of microscopic flow patterns is conducted.

Based on the analysis of a large number of simulations, we propose a correlation for shift factor which is quantified by the product of one fluid property parameter and tortuosity. The fluid property parameter is obtained from the analytical/semi-analytical solutions of the same shear-thinning fluids flow in a smooth slit. Two approaches are provided for tortuosity quantification. One is based on the detailed pore-scale velocity field and produces a very accurate shift factor. The other is the geometric tortuosity obtained by image analysis without doing any pore-scale simulations, which provides an approximate value for shift factor. The Forchheimer’s equation with our newly improved shift factor
correlation can be used in the higher-level macro-scale simulators to direct the relevant industrial applications.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-D / 405

4D-μCT analysis through piecewise linear fitting

Author(s): Marjolein Heyndrickx¹

Co-author(s): Matthieu Boone ¹; Thomas De Schryver ²; Tom Bultreys ³; Wannes Goethals ¹; Glenn Verstraete ¹; Valérie Vanhoorne ¹; Luc Van Hoorebeke ¹

¹ Ghent University
² XRE nv
³ Imperial College London

Corresponding Author(s): marjolein.heyndrickx@ugent.be

4D-μCT is an increasingly popular tool to study dynamic processes in situ, for example in material science and porous media studies. The technique allows to resolve changes in a material’s microstructure over time and in three spatial dimensions. Typically, a sample is scanned continuously during a relevant time-span, corresponding to multiple sequential conventional μCT scans, which are reconstructed and processed (analyzed) separately afterwards. However, the individual reconstructions of 4D-μCT scans often suffer from noise and motion artefacts. Also, the full dataset contains a temporal correlation which is typically not being exploited. In this presentation, we propose to use piecewise linear fitting, which starts from the low quality reconstructions and performs a piecewise linear fit in the time direction for each voxel. Despite yielding an improved contrast-to-noise ratio in every individual reconstruction, the technique does not introduce spatial blurring. Additionally, the technique results in a parametrization of the temporal domain, which can be directly used to analyze the dynamic process under investigation.

This piecewise linear fitting technique is applicable for a broad range of applications. It does not require prior knowledge, but can be adapted to exploit prior knowledge where it is available.

The technique is demonstrated on complementary samples from geological and pharmaceutical applications. The results show the improvement in the contrast to noise ratio and the potential to use the results in the further data analysis which needs to be performed after the reconstruction.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-C / 466

A C++ parallel solver for flow in networks of fractures

Stefano Berrone ¹; Alessandro D’Auria ²; Sandra Pieraccini ²; Stefano Scialo ²; Fabio Vicini ²

¹ Politecnico di Torino, Italy
² Politecnico di Torino
Corresponding Author(s): fabio.vicini@polito.it

The present work deals with the highly efficient parallel implementation of an optimization-based solver for the flow in Discrete Fracture Networks (DFNs). A DFN is a set of mutually intersecting planar polygons in the three dimensional space, resembling a system of fractures in the subsoil. Fracture networks are stochastically generated to tackle uncertainty and lack of observations on geometrical properties of the fractures (density, orientation, size) and on hydraulic properties (transmissivity). These random networks can be extremely complex, with a large number of fractures and intricate intersections, such that conventional simulation approaches have limited applicability in this context, mainly for the necessity of generating a conforming mesh of the whole network.

Recently a novel approach was presented to overcome the issue of mesh conformity in DFN flow simulations [1 2 3 4 5]. The method is based on the PDE-constrained minimization of a cost functional, which is introduced to handle matching conditions at fracture intersections with non conforming meshes. The minimization of the functional can be performed via a conjugate gradient approach, and the computation of the descent direction at each iteration of the method only asks for the resolution of small linear system on each fracture of the network. This structure naturally leads to a parallel approach. Here details on the implementation of this approach in the C++ language on distributed memory devices is discussed. The code aims at minimizing the number of communications among different processes, and the communication phases are organized in order to maximize the time occurring between the delivery of the data to their reception, thus shadowing the communication overhead.

References:


Click here to agree

Parallel 9-E / 712

A Computational Investigation of Seismic Wave Focusing as a Means to Fracture Shale

Rami Younis1, Yuxuan Jing1

1 University of Tulsa

Corresponding Author(s): yuj474@utulsa.edu

In unconventional oil and gas reservoirs, hydraulic fracturing can only generate fractures in limited bulk of reservoirs. Moreover, natural and hydraulic fractures are difficult to characterize, and the water disposal process is linked to environmental concerns including induced seismicity. Recent laboratory efforts report on the application of shock-wave comminution to micro-fracture considerable target bulk volumes of various porous materials such as limestone and concrete. The physical process is similar to lithotripsy; a widely applied kidney-stone treatment procedure. Few studies of rock comminution have been conducted at reservoir conditions. This work 1) develops a coupled seismic-flow simulation model that can predict the initiation of comminution at reservoir conditions, 2) applies the model to design laboratory rock mechanics experiments, and 3)
computationally investigates field-scale applications. We develop a high-resolution, coupled multiphase flow and transient geomechanics simulator for shale comminution. An unstructured, fully-implicit finite-volume formulation of the coupled equations is proposed in two-dimensions. In this model, the matrix rock is treated as a continuous porous medium and Biot’s theory is used to describe the bulk momentum balance. Wells are represented as internal boundaries within the mesh. Periodic or aperiodic deformations may be applied in addition to fluid injection and production. Strain energy release rates are computed and are used to judge the crack initiation and comminution processes. The simulator is validated numerically for accuracy and correctness and is compared to analytical solutions for simple cases. An investigation is conducted to design rock mechanics laboratory experiments that are projected to span the comminution onset and failure regimes. By controlling the generated seismic waves, comminution can be achieved in our model and can be controlled to initiate at intentional target locations. Compared to hydraulic fracturing that can only stimulate volumes near the wells, seismic waves can generate larger fractured volumes in target locations away from the wells. These preliminary results are encouraging and provide guidance to the development of next steps in the laboratory. A computational assessment shows that seismically induced comminution maybe realizable at reservoir conditions. A protocol to examine this in a laboratory setting is proposed. Seismic wave comminution may be a novel technology that will complement hydraulic fracturing in increasing recovery efficiency from unconventional reservoirs.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-G / 1012

A Computational Model for Freezing and Thawing in Soil

Mehdi Musivand Arzanfudi\textsuperscript{1} ; Rafid al Khoury\textsuperscript{None}

\textsuperscript{1} Delft University of Technology

Corresponding Author(s): r.i.n.alkhoury@tudelft.nl

A thermo-hydro-mechanical (THM) finite element model is developed to simulate freezing and thawing in soil. The governing equations are based on averaging theory and include conservation of mass, momentum and energy. The constitutive models constitute the equation of state (EOS) for water, Clausius-Clapeyron relationship for cryogenic suction, and empirical relationship for the melting point depression and unfrozen water content. The model is capable of simulating all important phenomena occurring during soil freezing, including: freezing induced heaving, convective-conductive heat transfer, water flow to the freezing region, and porosity change due to cryogenic suction and solid deformation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-C / 575
A Discrete Element Approach in Modeling Proppant Transport in 3D Fracture Networks

Rui Kou1; George Moridis1; Thomas Blasingame1

1 Texas A&M University

Corresponding Author(s): kourui.pete@tamu.edu

Objectives/Scope:
The understanding of proppant transport plays a critical role in estimating propped fracture dimensions and performance. Existing models generally assume a vertical planar geometry, whereas the reality in the subsurface may be much more complex. We use the discrete element method to simulate field scale proppant transport in complex fracture networks. Our results show that sharply-angled fracture networks reduce fluid velocity and increase the particle-wall interaction. The combined effects can cause early settling of proppants, thus limiting their efficient placement and the fracture effectiveness.

Methods, Procedures, Process:
To calibrate our numerical model, we conducted two validation simulations that describe particle settling tests and laboratory proppant transport experiments. Through scoping calculations, we determined the correct drag force model and matched both analytical solutions and experimental data for a wide range of flow regimes that included three proppant sizes (20-30 mesh, 30-40 mesh and 50-70 mesh) in two types of fluids (water and oil).

For the main component of our study, we simulated proppant transport in a 3 dimensional, field-scale fracture network using our benchmarked models. In our search for an optimal stimulation strategy, we also experimented with various perforation and pumping strategies, and then compared the proppant distribution results.

Results, Observations, Conclusions:
By analyzing the velocity and trajectory of proppant particles during transport, we identified two different stages of the proppant transport process — a “suspension” stage and a “settling” stage. During the suspension stage, the fluid drag and the gravitational forces dominate, driving proppants further into the fracture. When the proppants reach a flow stagnation area, or if/when the proppants collide with the fracture boundaries (side walls or bottom of fracture), the proppant particles lose momentum and then accumulate into “dunes” and become “settled.” Finally, we observed that proppant transport in a sharply-angled fracture network leads to local flow velocity reduction and stronger particle collision interactions, leading to dramatic reductions in the transport efficiency.

Application/Significance/Novelty:
This work provides a better understanding of proppant transport behavior in sharply angled fracture networks. A significant difference from prior (laboratory) experiments is the capability of our model to simulate proppant transport at field-scale flowrates. Such a capability is critical for understanding the proppant transport behavior by ensuring that the correct Reynolds number and flow regime are used in the calculations. To the best of our knowledge, this is the first study that emphasizes the importance of particle Reynolds number to proppant transport process.

Lastly, using the discrete element method and high-performance (parallel) computing, we were able to represent various perforation and pumping schemes, which is essential for developing an optimized stimulation strategy.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 816

A Dual-Continuum Hydromechanical Framework for Modelling Fractured Porous Media
Author(s): Mark Ashworth

Co-author(s): Florian Doster ; Sebastian Geiger

1 Heriot-Watt University

Corresponding Author(s): ma174@hw.ac.uk

A general framework for modelling hydromechanically coupled fractured porous media is implemented utilising the dual-continuum concept. Modelling fractured systems explicitly can be impractical at the field scale due to the size of the computational problem. Additionally, fracture properties are often not known unless directly accessed. The dual-continuum approach offers a practical method of gaining insight into the behaviour of fractured porous media over field scales. Previous numerical implementations of coupled dual-continuum models have all been implemented within equal-order mixed finite-element frameworks. Such frameworks are known to suffer instabilities due to failure to satisfy the Ladyshenskaya-Babuška-Brezzi (LBB) stability condition. The current framework makes use of a mimetic-type finite element method called the virtual element method for the mechanical problem, and the finite volume method for the flow problem. Similar approaches to the present have been shown to implicitly satisfy the stability condition, and to honour local mass conservation. Within reservoir engineering, coupled simulation is often done using dedicated software to model each subproblem. Coupling is then achieved by iterating between the mechanical and fluid subproblems. We make use of the iterative coupling approach and show that solving the coupled dual-continuum problem is not limited to the monolithic strategy used in previous implementations. Within the literature, there exist various approaches to formulating hydromechanically coupled dual-continuum models. These approaches can be grouped as phenomenological, thermodynamical, and microporomechanical accordingly. With our general framework we review different hydromechanically coupled dual-continuum models arising from these different methodologies.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 390

A Dual-site Simplified Local Density Model for Shale Gas Adsorption under Reservoir Conditions

Sen Wang ; Qhong Feng ; Farzam Javadpour ; Ming Zha

1 China University of Petroleum (East China)
2 The University of Texas at Austin

Corresponding Author(s): wangsen1@126.com

Direct measurement of shale gas adsorption isotherms at high pressures and high temperatures (HPHT) is intricate and requires expensive apparatuses. Most of the documented studies only report shale gas adsorption data at pressures below 12 MPa, which is much smaller than the reservoir pressure, e.g., up to 36 MPa in Eagle Ford shale. Recent studies also suggest that the excess adsorption isotherm of shale gas exhibits distinct features from that observed at low pressures. Therefore, predicting gas adsorption isotherms at reservoir conditions may be useful.

On the basis of the simplified local density (SLD) theory, we developed a novel dual-site adsorption model for shale gas. Shale matrix composed of both organic matter and inorganic minerals and the pores located within kerogen can be smaller than inorganic pores. Our grand canonical Monte Carlo (GCMC) simulations also confirm that the adsorption capacity of organic matter is much greater than those of inorganic minerals. Therefore, the model for shale gas adsorption isotherms should distinguishes methane adsorption in kerogen surface from that of the inorganic substrates. Our proposed dual-site SLD model takes into account the different pore sizes and fluid-solid interaction energy parameters of organic matter and inorganic minerals.

We first used conventional SLD model to match the excess adsorption isotherms of CH4 in graphene
and montmorillonite slt (pressure: 0-40 MPa). Excellent agreements are observed, which manifest that the SLD model is able to describe gas adsorption in a slt at both subcritical and supercritical states. Then we examined the validity of our proposed dual-site model using high-pressure CH4 adsorption isotherms on shale reported in the literatures. These experimental data were measured at pressures up to 25 MPa and temperatures up to 150 °C. Our proposed model fit these adsorption isotherms very well. If we use the experimental results measured at low pressures (~12 MPa) to make the fit, the high-pressure isotherms predicted using the fitted parameters are very close to the measured data, which demonstrated the validation of our model.

We also probed the differences of original gas-in-place (OGIP) and production performance estimated using low-pressure adsorption isotherms (always characterized using the Langmuir adsorption isotherms) and high-pressure adsorption isotherms. The great derivations suggest that reliable adsorption isotherms of shale gas under reservoir conditions are very essential. Our proposed dual-site SLD model provides an alternative method to predict shale gas adsorption isotherms under reservoir conditions using low-pressure experimental measurement.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 28

A Higher-Order Central-Upwind Scheme for Multiphase Flow in Heterogeneous Porous Media

Maicon Correa¹; Marcio Murad²

¹ Universidade de Campinas
² LNCC - Brazil

Corresponding Author(s): maicon@ime.unicamp.br

One of the most challenging issues in computational poromechanics is the development of numerical schemes capable of capturing in an accurate fashion the effects of spatial variability in the formation properties by handling highly heterogeneous coefficients with complex spatial distributions while preserving local conservation properties. In this work we present a new higher order semi-discrete central-upwind scheme for systems of conservation laws which allows for spatial heterogeneity of the storage coefficient, say, the porosity field. The proposed scheme adopts an inhomogeneous dual mesh with variable cell size ruled by one-sided local propagation speeds, which are used to construct the local Riemann fans and compute numerical fluxes at cell edges as in extending the results of [2] and [3], where the central scheme of [4] was used as basis for simulating multiphase flows in porous media. We also propose the use of the new central-upwind scheme in the composition of a sequential splitting algorithm for simulating incompressible multiphase flow within rigid and compressible porous media, with both permeability and porosity fields heterogeneous. Numerical tests are presented to illustrate the accuracy of the proposed method in problems that simulate immiscible three-phase flow in heterogeneous porous media in two and three space dimensions.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-G / 37

A Lagrangian scheme to model subgrid-scale mixing in heterogeneous porous media

Albert Valocchi1; Paulo Herrera2; Joaquin Cortinez3

1 University of Illinois at Urbana-Champaign
2 Independent Consultant
3 Arcadis Chile

Corresponding Author(s): valocchi@illinois.edu

Small-scale heterogeneity of permeability plays a major role in the spreading and mixing of contaminant plumes in groundwater systems. Spreading and mixing are interrelated because heterogeneity-induced spreading leads to the stretching of interfaces of the contaminant plume, while mixing across the interfaces is governed by local hydrodynamic dispersion. In many practical problems, mixing is the key process since it controls peak contaminant concentrations and overall rates of reaction during engineered or in-situ remediation. In spite of advances in high performance computing, it is still not possible to resolve all spatial heterogeneity scales in numerical simulation of conservative and reactive transport. We propose a Lagrangian numerical approach to implement closure models to account for subgrid-scale spreading and mixing in Darcy-scale numerical simulations of solute transport in mildly heterogeneous porous media. The novelty of the proposed approach is that it considers two different dispersion coefficients to account for advective spreading mechanisms and local scale dispersion. This technique considers fluid particles that carry solute mass and whose locations evolve according to a deterministic component given by the grid-scale velocity and a stochastic component that corresponds to a block-effective macro-dispersion coefficient. Mass transfer between particles due to local-scale dispersion is approximated by a meshless method.

Using results of benchmark numerical simulations, we demonstrate that the proposed approach is able to model subgrid-scale spreading and mixing provided there is a correct choice of block-scale dispersion coefficient. We assume for convenience the common adopted model that the hydraulic conductivity is a second-order stationary, log-normally distributed random field with exponential covariance. This allows use of the closed-form expressions for the block effective macro dispersion coefficient developed by Rubin and co-workers1 for the case of small variance. The presentation will be based on our recently published paper [2].

References:


Acceptance of Terms and Conditions:
Click here to agree
Poster 3 / 359

A Linear Domain Decomposition Method for Unsaturated Flow in Porous Media

Christian Rohde¹, David Seus², Florin Radu², Koondanibha Mitra³, Sorin Pop⁴

¹ University of Stuttgart
² University of Bergen
³ Eindhoven University of Technology
⁴ Hasselt University

Corresponding Author(s): k.mitra@tue.nl

The Richards equation is a commonly used model for unsaturated flow through porous media. Using the Darcy law in the mass balance equation, and bringing the resulting equation to a dimensionless form one obtains:

\[ \begin{align*}
\phi \partial_t S &= \nabla \cdot \left( \frac{K(S)}{\mu} \nabla p \right) + f(S, \nabla \phi) \\
\end{align*} \]

Here \( \phi \) is the porosity of the medium; \( z \) is the height; \( \rho, \mu \) are the density and the viscosity of water respectively. The nonlinear function \( K_r(S) \) (Relative permeability) is determined based on experiments and \( K \) (Absolute permeability) can vary in space. Two unknowns are involved: \( S \), the saturation and \( p \), the pressure of water. Commonly, it is assumed that these are related by a nonlinear relationship which is again determined based on experiments:

\[ \begin{align*}
p &= P_{ct}(S) \\
\end{align*} \]

The exact form of these nonlinearities depend on the medium. Most realistic problems involve heterogeneous media. Example in this sense are layered or fractured oil and gas reservoirs. In this case, the functions themselves are changing depending on the location inside the medium. In particular, if the adjacent blocks are separated by a fracture then this poses difficulties for the numerical simulation as generally different spatial discretization, models and pre-conditioners are used inside the fractures than in the blocks.

In this work we consider a medium consisting of \( N \) homogeneous sub-domains and propose a non-overlapping domain decomposition scheme that couples the models in the whole domain. The scheme involves linear iterations [Pop et al (2004), List and Radu (2016)]. Within one iteration the sub-domains are completely decoupled and are solved independently [Seus et al. (2017)]. After analyzing its convergence, we show some numerical results confirming the theoretical findings and discuss different implementation aspects.

References:


Click here to agree

Parallel 10-C / 233

A Meshfree Approach to Modeling Hydraulic Fracturing in Saturated Porous Media
Author(s): Haoyan Wei

Co-author(s): Jiu-Shyan Chen

1 Department of Structural Engineering, University of California, San Diego
2 Department of Structural Engineering, University of California, San Diego

Corresponding Author(s): h4wei@eng.ucsd.edu

The complex fluid-solid interactions and irregular crack patterns in hydraulic fracturing cause substantial numerical challenges, which can make conventional crack modeling methods ineffective. In the present work, a stabilized and nodally integrated meshfree formulation for hydro-mechanical modeling of crack propagation in saturated porous media is developed. Under the stabilized conforming nodal integration framework [1], a fluid pressure projection method [2] is employed to achieve a stable equal-order reproducing kernel approximation for the mixed poromechanical formulation. Furthermore, a damage particle method is proposed, which approximates the fractures by a set of damaged particles under the meshfree discretization. For each damaged particle, a continuum damage mechanics model is adopted as a smeared type description of the equivalent crack segment at the nodal position, and a dissipation energy-based scaling law is naturally introduced to enforce the bulk energy dissipated over the nodal quadrature cell to be consistent with the surface fracture energy of the equivalent crack segment. A simple tracking procedure for damaged particles is employed to prevent spurious damage initiation and spread, and thus the global energy dissipation is conserved. In addition, the influence of cracking on the fluid flow is captured by adopting a cubic law-based anisotropic permeability model, which is updated during the simulation by extracting the equivalent crack opening displacement from the damage and deformation field. The proposed reproducing kernel damage particle method provides an effective means in modeling fluid-driven propagating cracks. Several numerical examples are given to demonstrate the effectiveness of the developed meshfree formulation.

References:

Click here to agree

Poster 2 / 438

A Model for Gas Transport in Inorganic Nanopores of Shale Gas Reservoirs

Author(s): Shan Wang

Co-author(s): Juntai Shi; Chenhong Hou; Yucui Chang

Corresponding Author(s): wsocupb2016@163.com

The shale gas reservoirs are rich in organic and inorganic nano-sized pores. Generally, both adsorbed gas and free gas are considered to be exist in organic matrix pores, while there is no adsorbed gas in inorganic matrix pores. Therefore, gas transport mechanism is quite different in these two types of nanopores. Many researchers have provided the presence of water film on the inorganic pore surface due to its strong hydrophilic ability. However, most of the models for gas transport in shale inorganic nanopores ignore the effect of water distribution on gas transport, which lead to overestimating of gas transport capability.

In this paper, a new gas transport model for inorganic nanopores in shale gas reservoirs is proposed. First, considering the gas transport capability varies with pore size, the logarithmic normal distribution function is utilized to describe the nanopores distribution in shale inorganic porous media. Then, the influence of real gas effect, stress dependence and water distribution are all considered to derive the model. The validation results show that the proposed model and published experimental data can be well fitted. Finally, the effect of each factor on gas transport capability in shale inorganic...
nanopores is analyzed and discussed. The results indicate that the gas transport capability will decrease with the increase of relative humidity. When the relative humidity increases to a critical value, the nanopores will be blocked with capillary water. During depressurization development process, the effective pore size will apparently reduce due to the influence of stress dependence, which cannot be ignored. Furthermore, when the shale inorganic matrix pores have the same mean pore size, the gas transport capability under various pore distribution probability is quite different, and the lower the peak frequency, the higher the transport capability. Meanwhile, under high temperature and low pressure conditions, methane transport capacity is significantly higher than ethane and carbon dioxide. The research results of this paper can provide a reference for the analysis of nanoscale gas flow mechanism in shale matrix, and also provide a theoretical basis for more accurate production prediction of shale gas wells.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 803

A Molecular Dynamics Approach for Predicting the Glass Transition in pores

Elena Kirova¹; Norman Genri²; Vasily Pisarev³

¹ HSE

Corresponding Author(s): kirova@phystech.edu

Molecular dynamics study of the glass transition process in metallic glasses is performed. As an example, the liquid aluminum film is taken. The embedded atom method potential is used at the simulation of isobaric cooling [1]. There is a number of glass transition criteria: the decrease of the specific heat of material (calorimetric criterion) [2], the splitting of the second peak of the pair correlation function and the icosahedral short-range order (structural glass transition criteria) [3], the change of diffusivity behavior (dynamic criterion). However, the difference between the calorimetric glass transition temperature and the temperature, obtained using the structural and dynamic criteria might reach several hundred kelvins [4]. In the current work we obtain the glass transition temperature using two methods based on the shear stress correlations behavior. The first method is based on the stress correlations in the plane of the film and the steep change of the kinematic viscosity, obtained using Green-Kubo formula. The second method is based on the transverse oscillations in the film. The glass transition temperature is estimated from the temperature dependence of the oscillation damping of the stress correlation functions. The increasing in the kinematic viscosity correlates with the decrease of transverse oscillations damping in the film [5]. The obtained glass transition temperature agrees with the calorimetric temperature. Also, the temperature when the system becomes non-equilibrium is estimated, which is also in a good agreement with the obtained results.

The new methods of obtaining the glass transition temperature are validated on a metallic melt which is in contact with the walls. As an example, the Al-Fe alloy between titanium walls is taken. The embedded atom method potential is used to simulate titanium-aluminum systems, the Finnis-Sinclair embedded atom method potential is used for describing the interaction between Al and Fe. The interaction between Ti atoms is described by the Modified Embedded Atom Method potential. The alloy is cooled by changing the walls temperature. The glass transition temperature is obtained using the glass transition criterion based on the transversal sound propagation. Also, the viscosity behavior is considered. The dependence of the glass transition temperature on the pore size is obtained.

The authors acknowledge the Supercomputer Center JIHT RAS and Joint Supercomputer Center of the Russian Academy for providing computing time. The study has been funded by the Russian Academic Excellence Project "5-100".

References: 


Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 457

A New Dynamic Single-Pressure Network Model: Experimental Comparisons and Calibrations.

Author(s): Morten Vassvik
Co-author(s): Magnus Aa. Gjennestad; Alex Hansen

1 Department of Physics, Norwegian University of Science and Technology
2 Norwegian University of Science and Technology
3 NTNU

Corresponding Author(s):

We present a simple single-pressure dynamic network simulator for two-phase flow in porous media with a focus on exploring the limits of a single-pressure network model.

Our work builds upon the work of Aker et al. [3] and Knudsen et al. [2], where we aim to more accurately describe and model the interactions of ganglia moving through the porous material. Whereas the previous models assumed constant cross-section pipes, we instead account for a varying cross-section along a pipe. This is important as the size of trapped wetting bubbles is determined by both the throat size and the pore size, and are over-predicted for straight pipes.

Another focus is on accurately modelling the interaction of ganglia across adjacent pipes. This is the dominant mechanism that determines the ganglion size distribution in the network - a ganglion cannot split below the size of a pore for sufficiently slow flow rates.

Our model is of the single-pressure kind, where only one phase can occupy a cross-section at a time. Consequently we neglect wetting fluids in films and corners. One aim of our study is to investigate the limits of a simple single-pressure network model without resorting to a much computationally heavier two-pressure model [5]. This excludes us from modeling strong imbibition invasions where the main transport mechanism is dominated by film and corner flow.

We will present direct comparisons to drainage and mixed-wet invasion studies by Zhu et al. [4], and to experiments by Moura et al. [5, 6] studying the burst dynamics of an invasion process. In addition we will present some qualitative comparisons to the experimental work of Avraam and Payatakes [7] on the dynamics of ganglia.

References:

A New High-fidelity Mesh Model for Simulation of Transport Process in a Fixed Bed Reactor

Author(s): Bing Yuan
Co-author(s): Junbo Xu, Yongqi Zhang, Chao Yang

1 College of Chemical Engineering, Sichuan University, Chengdu 610065, China; CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, University of Chinese Academy of Sciences, Beijing 100190, China
2 CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, University of Chinese Academy of Sciences, Beijing 100190, China
3 SINOPEC Research Institute of Petroleum Processing, Beijing 100083, China
4 College of Chemical Engineering, Sichuan University, Chengdu 610065, China; CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

Corresponding Author(s):

The traditional fixed-bed reactor design is usually based on empirical correlations of plug flow pattern. This empirical method is usually not suitable for the low tube-to-particle diameter ratios (N=D/d< 4) where the local phenomena of channeling near the wall and the backflow in the bed are dominant. The recent “solid particle” method is too complicated for mesh generation, especially for large random packed beds, which seriously hinders its development. In this work, a novel mesh model is proposed and used for the simulation of fixed bed reactors by combining discrete element method with the user defined subroutine. The mesh generation process is simple and easy to be implemented, which ingeniously avoids handling the complex “contact point” problem. In this study the packed beds with spherical and cylindrical particles are investigated, the local flow in the bed can be high fidelity. The predictions of the pressure drop across the fixed bed and the heat transfer of the single particle are in good agreement with the corresponding empirical relations.

Acknowledgement

Financial support from the National Key Research and Development Program (2016YFB0301702), National Natural Science Foundation of China (21490584, 91534105, Major National Scientific Instrument Development Project (21427814) and Key Research Program of Frontier Sciences of CAS (QYZDJ-SSW-JSC030) is gratefully acknowledged.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 988

A New Method for Estimating the Clay Content of Tight Oil Reservoirs from NMR Logs
Author(s): Ziyue Li¹ ; Zhiqiang Mao³
Co-author(s): Yujiang Shi² ; Jinhua Fu ; Peiqiang Zhao³

¹ State Key Laboratory of Petroleum Resources and Prospecting, China University of Petroleum, Beijing, 102249
² National Engineering Laboratory for Exploration and Development of Low-Permeability Oil & Gas Fields, PetroChina Changing Oilfield Company, Xi'an 710018, China
³ Institute of Geophysics and Geomatics, China University of Geosciences, Wuhan

Corresponding Author(s): liziyue1209@126.com

Due to the differences in physical properties between clay mineral and sand matrix, clay content has always been an important part of reservoir evaluation. Clay content can be used to calculate effective porosity, saturation and permeability in conventional reservoirs and provide available information for brittleness evaluation and hydraulic fracturing design in tight oil reservoirs or shale gas reservoirs. However, anomaly high value of gamma-ray logs and low resolution of spontaneous potential logs in source-reservoirs make it difficult to calculate clay content. What’s more, the calculation of clay content is lack of precision even through optimization method because of the extremely complex lithology of source-reservoirs.

This paper proposed a new method for determining the clay content of tight oil reservoirs of Lucao-gou formation in Jimusaer Sag, Junggar Basin using the NMR logs. Four kinds of sandstone samples with different types of clay minerals and the target tight oil rock samples have been analyzed by X-ray diffraction and NMR measurement. The results indicate that the T2 peaks of centrifuged samples with illite and/or montmorillonite are below 10ms, and that the T2 peaks of centrifuged samples with kaolinite and/or chloride are greater than 10ms, or even 20ms. This is accord with the experimental results about T2 relaxation time of different clay minerals presented by previous research. Different types of clay have different specific surface areas and relaxivities. Thus, the T2 cutoffs for clay bound water vary with the clay types. Based on the results, T2 cutoff of specific clay minerals determined by NMR method can be used to calculate clay water saturation. The relationship between clay content, clay water saturation, and density logs in the study area is established through the equation for cation exchange capacity and clay water saturation. Then we use least square method to set up a statistical model of clay content according to this relationship. The clay mineral contents of Lucao-gou formation calculated by this model yield a good agreement with those obtained by experimental measurement, thus verifying the effectiveness and reliability of the proposed method.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 491

A Novel Mehtod to Correct Steady-State Relative Permeability for Capillary End-Effects Based on Simulation Approach

Shiyuan Zhan¹ ; Yuliang Su² ; Wendong Wang² ; Mingyu Cai¹ ; Dongxia Li³

¹ School of Petroleum Engineering, China University of Petroleum (East China)
² China University of Petroleum (East China)

Corresponding Author(s): zhanshiyuan321@163.com

In laboratory steady-state measurements of relative permeability, capillary discontinuities at sample ends give rise to capillary end-effects (CEE) and keep a higher water saturation toward the core end. The water saturation measured is higher than ideal saturation without CEE and result of erroneous relative permeability curve finally. Especially in tight sand cores, high capillary force and low flow rates can cause end-effects to become more important in the interpretation of the steady-state experiment tests.

On the basis of capillary force measurement data, a novel method was initiated to make correction to relative permeability data combined experiment data and numerical simulation for tight sand
cores. First, one dimensional numerical simulator was created for oil and water two phase flow considering the mechanism of CEE. Water saturation distribution and CEE region could be clarified corresponding to the relative permeability curve input. And then correct relative permeability input constantly until the average water saturation simulated consistent with the saturation measured by experiment. The new method could make correction to relative permeability based on the traditional experiment data of multiple fractional flow and same total flow rate, which is more practical than “intercept method” [3]. The impact of end-effects and practical means of reducing the end effects for tight sand cores are also discussed in this paper.

References:


Click here to agree

Poster 4 / 299

A Numerical Method of Coupled Reservoir-Geomechanical Problem Using High Resolution for Fluid Flow Domain

Dawei WU¹ ; Yuan Di¹ ; Yun ZHANG² ; Zhongchun LIU²

¹ Peking University
² Exploration & Production Research Institute, SINOPEC

Corresponding Author(s): daweiwu@pku.edu.cn

Accurate prediction of petroleum reservoir production in structurally weak geologic areas such as fractured reservoirs or low-permeability reservoirs requires both mechanical deformation and fluid flow modeling. Even production of reservoirs located in stable environments may also need to be predicted by fluid-solid coupled models in case of injection of water or carbon dioxide. The equations governing the interaction of solid and fluid in rocks are equilibrium equation and continuity equation. Generalized finite element method is usually adopted for the fluid-solid coupled models, however it needs rather much effort in programming and is not satisfactory in computational efficiency. The mixed finite element and finite volume scheme is proposed as an alternative method since it involves less computational effort and improves the simulation efficiency. In the mixed FEM-FVM method, the equilibrium equation is discretized in the spatial domain for geomechanics by finite element method, and the continuity equation is discretized in the fluid flow domain by finite volume method. Solving this coupled set of equations, the displacement of solid and pore pressure can be obtained.

In the actual simulation of reservoir exploitation, the fluid flow should only be simulated in the reservoir area, while the geomechanics need to be investigated in the whole computational domain up to the ground in order to fully capture the effect of stress and strain change on fluid flow. Thus the flow domain is typically a subset of the geomechanics domain. In some coupled analysis, additional computational domains are added above and below the reservoir area known as overburden and underburden in order to better capture the stress field. However, these extra domains significantly increase the computational cost of simulation. Moreover, how large area of overburden and underburden is needed to fully capture the stress change still needs further investigation.

In order to improve the computational efficiency of coupled analysis when overburden and underburden computational domains are included, a FEM-FVM method using high resolution for fluid flow domain is proposed in this paper. The advantage of the presented method is that different computational grids could be used for finite element method and finite volume method. The grids used in finite volume method are set up by meshing inside the finite element grids for fluid flow domain. Therefore numerical simulation of fluid flow can be carried out in finer resolution for reservoir domain when geomechanics simulation will be carried out in coarser grids. Since the geomechanics
component causes most of the calculation burden, this method can significantly improve the efficiency of the whole simulation. Several numerical examples are presented to show accuracy and efficiency of the proposed method.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-C / 76

A Practical Scale-Up Workflow for Numerical Simulation of Post-CHOPS (Cold Heavy Oil Production with Sand) Solvent-Aided Processes

Juliana Leung

1 University of Alberta

Corresponding Author(s): juliana2@ualberta.ca

Cold Heavy Oil Production with Sand (CHOPS) is widely used as a primary non-thermal production technique in thin heavy oil reservoirs. Development of the complex wormhole networks (i.e., high-permeability channels caused by sand production) renders the scalability of post-CHOPS solvent-aided processes to field applications challenging. It is widely accepted that configuration of wormhole networks and foamy oil flow are key characteristics pertinent to these processes.

First, a series of mechanistic compositional simulation models at the lab scale is constructed to model a cyclic solvent injection scheme (CSI). These models are calibrated against experimental measurements of solvent diffusion measured in porous media. Next, a set of detailed high-resolution (fine-scale) simulation models, where both matrix and high-permeability wormholes (modeled as fractal networks) are represented explicitly in the computational domain, is constructed to model how the solvent propagates away from the wormholes and into the bypassed matrix. Finally, a statistical scale-up procedure is developed to assign parameters of the equivalent dual-permeability model (e.g., dispersions, shape factors) in accordance to the grid size and wormhole intensity within the grid block. The novelty of this scheme is that the bivariate distributions between effective dispersivities and wormhole intensity at the coarse scale are calibrated from detailed fine-scale simulations.

In the end, field-scale simulations are constructed using average petrophysical and fluid properties extracted from several existing CHOPS reservoirs. Wormhole development and the end state of CHOPS are modeled using the concept of critical pressure gradient. Multiple field injection scenarios (i.e., of different number of cycles and durations of the soaking period) are analyzed. As expected, extended soaking period is more beneficial in terms of ultimate oil recovery, but it also reduces the early production rate. Interestingly, when an economic limit (i.e., minimum oil producing rate) is imposed, the optimal soaking time is not necessarily the longest one. It depends on the trade-off between extracting additional oil recovery at late times versus producing at a higher rate at early times. Our results also support the strategy of injecting all the solvent in one single consolidated cycle, with an extended soaking period, rather than performing shorter consecutive cycles.

Field-scale flow simulations are often performed to approximate the reservoir response and to optimize operating strategies. However, grid block sizes in field-scale models are generally much larger than the wormhole scale, and numerical analysis is often performed by arbitrary adjustment of dispersivity. This work, however, offers a statistical scale-up workflow that facilitates the construction of coarse-scale dual-permeability models, whose shape factors, fracture spacing, fracture porosity, and effective dispersivities are assigned based on calibration against simulation results of detailed fine-scale wormhole network models. The proposed method serves as a starting point for formulating a systematic workflow that can be integrated with commercial reservoir simulators to effectively simulate solvent processes in wormhole networks that span over multiple scales.

References:
Acceptance of Terms and Conditions:
Click here to agree

**Poster 4 / 583**

**A Prediction of the Spatial Distribution of Petrophysical Properties with Bernstein Copula using Seismic Attributes as Secondary Variables**

*Author(s):* Martin Alberto Díaz-Viera¹ ; Van Huong LE²

*Co-author(s):* Daniel Vázquez-Ramírez ²

¹ *Instituto Mexicano del Petróleo*
² *UNAM*

*Corresponding Author(s):* mdiazv@imp.mx

One of the main objectives of oil reservoir geological modeling is to predict the spatial distribution of petrophysical properties from a few poorly distributed data. To achieve this goal, it is usually necessary to establish some dependence model so that it is possible to predict petrophysical properties of interest through its relationship with seismic attributes that are more densely sampled. The usual models that are commonly applied to represent the dependencies between petrophysical properties and seismic attributes, are limited to linear or empirical correlations that, due to their simplicity, do not adequately capture the complex dependency relationships that exist between them, underestimating in most of the cases, the variability of the data and their extreme values.

In modern statistics, a systematic and flexible way of modeling complex dependencies is through copulas. Copulas are functions that allow to capture the relation of joint dependency between random variables independently of their individual marginal behavior.

In this work a method for spatial stochastic simulation of petrophysical properties with Bernstein copulas using seismic attributes as secondary variables is applied. The method basically consists of two stages, in the first one a Bernstein copula for dependency structure between the petrophysical properties and seismic attributes is modeling, while in the second one the spatial distribution of petrophysical property is simulated by including the relationship of dependence previously obtained applying the simulated annealing method. The resulting simulation method has among other advantages that it does not assume any probability distribution, it honors the hard data and reproduces the spatial correlation specified by the variogram.

The developed methodology was applied to a real case study for a deep water siliciclastic reservoir, obtaining highly satisfactory and competitive results when compared with regression techniques and traditional geostatistical simulation methods such as the Gaussian sequential simulation.

**References:**


Acceptance of Terms and Conditions:
Click here to agree

**Poster 3 / 826**

**A Semi-Analytical Model for Characterizing the Transient Flow Behavior of Reoriented Refractures Considering the Interference from the Initial Fractures**
Bailu Teng¹ ; Huazhou Li¹

¹ University of Alberta

Corresponding Author(s): bailu@ualberta.ca

In order to improve the field productivity, the industries can create new fractured wells to reduce the interval between the initial fractures. However, the production from the initial fractured wells can induce stress reorientation in the vicinity of the fractures. As such, a refracturing treatment in the stress reorientation region can lead to a reoriented refracture which has a more or less azimuth with respect to the initial fracture. This azimuth can even be 90 degrees if the stress reorientation is sufficiently large. Tiltmeter data monitored in the Lost Hills field and the Codell formation justify that the reoriented refractures can be frequently observed after the refracturing treatment. In addition to the refracture’s length, refracture’s conductivity and the in-situ conditions, there are two more factors, the reorientation azimuth and the interference from the initial fracture, can exert significant influence on the transient flow behavior of the reoriented refractures. In such case, the conventional analytical/semi-analytical models which neglect these two factors are no longer applicable to characterize the transient flow behavior from such a refracture.

In this work, we develop a novel semi-analytical model to characterize the transient flow behavior of a reoriented refracture considering the interference from the initial fractures. In this model, the fractures are explicitly represented with discretized segments. We apply finite difference approximation to the initial fractures and refractures, respectively, to simulate the transient flow in the fracture system. Additionally, the fluid flow in the matrix system can be characterized by Green function and Newman product principle. Based on the continuity of flux and pressure, we couple the fracture flow equations with the matrix flow equations to construct a semi-analytical model. Hereafter, we validate the proposed model against a commercial numerical simulator.

With the aid of the proposed model, we distinguish the flow regimes of a reoriented refracture on the dimensionless pressure derivative plot. These flow regimes include wellbore after flow, bilinear flow, formation linear flow, early pseudoradial flow and late pseudoradial flow. During the early pseudoradial flow period, the dimensionless pressure derivative plot is asymptotic to $y = 0.5$ on the log-log plot, whereas during the late pseudoradial flow period, the dimensionless pressure derivative is asymptotic to a value that is a function of the production rates of the initial fracture and the refracture. In addition, we carry out a thorough investigation about the influences of fracture conductivity, reorientation azimuth, position of the refracture, and production rate of the initial fracture, on the pressure response of a reoriented refracture. The interference from the initial fracture is studied at constant-production-rate constraint and constant-bottomhole-pressure constraint, respectively.

This proposed model can be applied to the real field cases in three different ways: first, one can use this proposed model to obtain the properties of the refracture by matching the historical production data; second, the performance of a refracture can be evaluated before the refracturing treatment in order to optimize the refracturing treatment; and third, one can use this proposed model to predict the production of a reoriented refracture once the properties of the refracture are known.

References:

Acceptance of Terms and Conditions:

Click here to agree
An ultra-tight sealing caprock is essential for safe storage of CO2 in deep geological basins. One of the basic requirements of this shale sealing is to ensure it is free of faults/fractures or other high permeable zones that may lead to unintended leakage of CO2 from its storage reservoir to above zones. Sealing capability of caprock is typically characterized by permeability measurement of a sample cored from the desired caprock formation. However, this does not ensure the presence of any faults/fractures or other high permeable zones in the caprock at field-scale. Characterizing a sealing caprock is a challenging task because dynamic data is not available from any region inside the caprock. However, monitoring data from above and below the caprock can be used for its characterization at field-scale. This study presents a method to stochastically characterize a sealing caprock (e.g. ultra-tight shale) using pressure monitoring data from above and below the caprock. This monitoring data is used in combination with other readily-available data from laboratory and outcrop in a history-matching optimization process to characterize the spatial variation in porosity and permeability of the caprock. An optimum geological model of caprock, representing a most-likely scenario, is selected from an ensemble of stochastic realizations generated using optimized parameters.

The method is demonstrated using four representative heterogeneous fractured seal types ranging from impermeable to highly permeable. The sensitivity to caprock thickness, pressure variation, and time length of monitoring data is also investigated.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-F / 410

A Terzaghi-Like Principle for Swelling Porous Materials

Lynn Schreyer¹

¹ Washington State University

Corresponding Author(s): lynn.schreyer@wsu.edu

Terzaghi’s Principle states that the total stress acting on a porous material can be decomposed linearly into a part that acts on the solid porous structure and the fluid pressure. The result of the Terzaghi’s Principle is that the stress-strain relationship for porous media does not have to be reconstructed for every possible fluid pressure – increasing the fluid pressure linearly affects the total stress. This Principle assumes there is only one fluid phase, the solid component and liquid are incompressible, the material is homogeneous, and the drained compressibility coefficient is constant throughout the range of strains (typically small strains). How should this be extended for swelling porous materials, where the liquid pressure is not directly measurable? Here we give a simple derivation, using total differentials and an appropriate choice of independent variables, and derive a Terzaghi-like principle for swelling porous materials.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 437
A Transient Productivity Model of Multi-stage Fractured Horizontal Wells in Shale Gas Based on the Continuous Succession Pseudo-steady State Method

Fanhai Zeng¹ ; Xiaowei Wang¹ ; Jianchun Guo¹ ; Botao Tang¹

¹ Southwest Petroleum University

Corresponding Author(s): zengfanhui023024@126.com

The multi-stage fractured horizontal wells (MFHW) is the key technology for developing shale gas reservoirs. After the stimulated reservoir volume is fractured, the gas flowing in matrix is non-linear seepage controlled by the nano-scale pores, while the seepage in stimulated region is transformed into Darcy flow controlled by the micro-scale fracture network. In this paper, the steady-state productivity model of MFHW is firstly established by comprehensively considering the multi-scale flowing states, shale gas desorption and diffusion after shale fracturing, which coupled flows in matrix and stimulated region. On this basis, for the first time, a transient productivity calculation model of MFHW combined the material balance equation is obtained with the continuous succession pseudo-steady state method (SPSS), which considered the unstable propagation of pressure wave. And the horizontal well productivity prediction and factors analysis are carried out by using the SPSS. The results show that the SPSS has the advantages of simple process of calculation, fast calculation speed and high agreement with numerical simulation results. During the production process, the desorption effect of shale gas is the key factor affecting the transient productivity of gas wells. During the production process, the desorption effect of shale gas is the key factor affecting the middle and late stage production of gas wells. With the increase of the radius and permeability of the mass fractures, the diffusion coefficient and Langmuir volume, the productivity of shale gas wells would increase, while the increasing rate would decrease. And the effect of Langmuir pressure on productivity is less. It is concluded that this method provides a theoretical basis for the calculation of transient productivity of shale gas fractured horizontal wells.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-D / 68

A Unified Viscous-Diffusion Layered Model of Non-ideal Rarefied Gas Flow in Micro- and Nanoscale Porous Media

Di Chai¹ ; Xiaoli Li¹

¹ University of Kansas

Corresponding Author(s): dchai@ku.edu

OBJECTIVES/SCOPE:
Existing rarefied gas flow models cannot accurately unify various flow mechanisms by empirical methods and overlook the van der Waals effect. In this paper, a model for non-ideal rarefied gas flow in nano- and micro-porous media is developed based on the well-recognized Bravo’s conceptual layered model with the rigorous interpretation. The gas transport behavior in nanopores can be simulated by the developed model which can be integrated with hydraulic fracturing models to optimize the production performance of shale gas reservoirs.

METHODS, PROCEDURES, PROCESS:
The cross-section of a nano-capillary can be divided into two zones based on Bravo’s model, i.e., an inner circular zone where the viscous flow behavior mainly exists due to the dominant intermolecular collision and an outer annular zone where non-equilibrium phenomenon exists and the classic constitutive relation breaks down due to a lack of intermolecular collisions. We proposed a virtual boundary between two zones which is determined by Kennard’s collision model, where the radius
of inner zone is correlated with the fraction of intermolecular collisions. The convective and
diffusive fluxes are rigorously integrated based on the virtual boundary. The mass flux, contributed
different transport mechanisms, thus could be analyzed by varying the Knudsen number. Sub-
sequently, non-ideality property of rarefied gas is characterized by incorporating a compressibility
correlation and real gas viscosity function. Physical and numerical experiments show the support
of the new formulation and provide approaches to obtain apparent permeability and a generalized
Klinkenberg’s parameter which is a function of Knudsen’s number.

RESULTS, OBSERVATIONS, CONCLUSIONS:
The newly proposed model allows for determination of the pressure dependence of the Klinkenberg
parameter across the transition flow regime and yields the most accurate prediction compared with
five existing models. The apparent permeability does not change obviously when pressure is over
10 MPa and pore size is larger than 100 nm. Although the surface roughness can significantly re-
duce the apparent permeability, its impact is minor when the pressure is higher than 10 MPa. The
molar gas flux declines significantly by incorporating the real gas effect into the model, leading to
a decreasing apparent permeability. Sensitivity analysis shows the apparent permeability is found
to be strongly dependent on pore size and weakly dependent on roughness. Finally, it is found that
Knudsen diffusion dominates the flow performance with a proportion larger than 60% in small pores
(e.g., ≤ 50 nm) at the low pressures (e.g., ≤ 0.2 MPa).

NOVELTY:
Instead of the empirical coefficients commonly used in most existing models, the weight coefficient
of viscous flow and Knudsen diffusion in the proposed layered model is analytically derived based on
Bravo’s layered model. This work also provides approaches to obtain a generalized Klinkenberg’s pa-
rameter. In addition, a multi-objective optimization method is adopted to enhance the conveniences
of searching local optimal fitting parameters in empirical correlations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-F / 417

A bottom-up approach to obtain continuum model parameters from pore network drying simulations

Xiang Lu1 ; Abdolreza Kharaghani1 ; Evangelos Tsotsas1

1 Thermal Process Engineering, Otto von Guericke University Magdeburg

Corresponding Author(s): abdolreza.kharaghani@ovgu.de

Several mathematical models with various degrees of complexity and accuracy have been developed
to describe the dynamics of drying porous media. At the effective medium scale, a continuum ap-
proximation is used and the transport phenomena are described by a set of partial differential equa-
tions. While classical and extremely useful, and in spite of many studies, the continuum models
(CMs) we have at our disposal are inadequate for various reasons. These CMs require macroscopic
transport parameters, which are averages of corresponding microscopic properties and are often
determined by laborious experiments. On the other hand, the microscopic models, which are able
to resolve the sub-pore scale physics, are far from being practical, either computationally or analy-
tically. In-between these two model hierarchies (macroscopic and microscopic), the mesoscale pore
network models (PNMs) have been developed extensively since recent years. The original intent of
PNMs for drying was to provide a relatively detailed picture and a fundamental understanding of
the pore-scale phenomena that occur in porous media during the drying process. Very recently we
have gone beyond this aspect: The parametrized version of the one-equation CM has been revisited
and assessed by PN simulations [2]. It has been realized that for drying of non-hygrosopic porous
media the classical interpretation of the relationship between the vapor partial pressure and the sat-
uration, which was introduced in the development of the CM by the desorption isotherm, is not true
[2]. In this work, three-dimensional pore network simulations of drying are carried out for several
pore structures with different geometrical and morphological properties. Significant differences in parameters are observed for variations in the network pore structure. For instance, the results show that the dependency of the vapor partial pressure on the saturation is not unique during the drying process, and it depends strongly on the pore structure. Finally, the ability of the CM to predict the PN simulation results for multiple realizations is explored. Our long-term vision is to derive new and superior continuum models from discrete drying simulations with realistic pore networks.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 680

A comprehensive simulation model for solvent-aided thermal recovery of heavy oil and bitumen—Analyzing the impact of diverse factors on productivity and product selectivity

Kyung Jae Lee

1 University of Houston

Corresponding Author(s): kjlee6@central.uh.edu

A new simulation model for solvent-aided thermal recovery of heavy oil and bitumen has been developed. The simulation model describes non-isothermal, multiphase, and multicomponent reservoir systems involving multiple kinetic reactions of heavy oil cracking. In the development of numerical simulator, we include 12 fluid-and-solid components in four phases of 1) aqueous, 2) liquid organic, 3) gaseous, and 4) solid phases. The 12 fluid-and solid components are 1) water, 2) heavy oil, 3) light oil, 4) asphaltene, 5) methane, 6) ethane, 7) propane, 8) hydrogen, 9) carbon monoxide, 10) carbon dioxide, 11) hydrogen sulfide, and 12) coke. It describes relevant physical and chemical phenomena during in-situ heating and production, such as dynamic changes of rock-and-fluid properties as a function of system conditions, phase transition thermodynamics, heat transfer by conduction and convection, pore clogging by coke generation from reactions, and porosity and permeability alteration. The application cases of numerical simulation are categorized into four as follows. Firstly, we conduct local sensitivity analysis of productivity and product selectivity to diverse uncertain parameters. They include reaction parameters, formation water saturation, and rock permeability. The effect of each parameter has been quantified, and the most influential parameters to the hydrocarbon productivity have been figured out. Product selectivity, especially for unwanted gases of carbon dioxide and hydrogen sulfide is analyzed, as being affected by uncertain parameters. The delivered most influential parameters are the most important data to be measured, to reduce the prediction uncertainty of unwanted acid gases of carbon dioxide and hydrogen sulfide. Secondly, we analyze the diverse heating methods. The heating methods include 1) electrical heating, 2) heating by hot water drive, 3) heating by hot water drive containing condensate, 4) electrical heating with hot water drive, and 5) electrical heating with hot water drive containing condensate. In each case, both physical and chemical changes of system are considered and compared, such as viscosity, density, and composition of the fluid phases; and optimized heating method for maximizing productivity has been figured out. Thirdly, we also quantify the effect of heating temperature to the productivity and product selectivity. High heating temperature activates the reactions of heavy oil cracking, but also accelerates the generation of solid product, coke. Here, the effect of pore clogging by coke generation to the permeability alteration and subsequently altering fluid flow and heat convection is analyzed. Through
a case study, we find an optimal heating temperature for maximizing productivity. Fourthly, we conduct the simulation runs using diverse ratios between condensate and water in the cases of hot water drive containing condensate. It is found that the optimal ratio between condensate and water is affected by the wettability of the porous media and initial water saturation. From the plentiful simulation cases, the optimization of in-situ heating and production in heavy oil and bitumen reservoirs has been realized. The developed simulator provides the powerful tool to investigate the impacts of various unknown parameters and controlling factors, and hence enables us to increase the success-likelihood of hydrocarbon production from thermally-cracked heavy oil/bitumen reservoirs.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-E / 917

A continuum model of gravity fingering endowed with an entropy function and bounded saturation overshoot

Abdelaziz Beljadid¹ ; Luis Cueto-Felgueroso² ; Ruben Juanes³

¹ MIT
² MIT and Technical University of Madrid
³ MIT

Corresponding Author(s): beljadid@mit.edu

Gravity-driven fingering is commonly observed during water infiltration in soil. An important feature of gravity fingering is the presence of saturation overshoot, which is understood to be a necessary prerequisite for gravity fingering in unsaturated flows. The Richards model in its basic form, along with the standard (monotonic) pressure-saturation relation, is incompatible with saturation overshoot for infiltration into unsaturated homogeneous media and cannot reproduce the fingering phenomenon.

Most model extensions of the Richards equation do not guarantee that the saturation overshoot be bounded. To remedy this unphysical situation, additional techniques have been invoked and incorporated into multiphase models, such as the use of a relaxation term (Nieber et al., 2005) or adding a compressibility term in the capillary potential (Cueto-Felgueroso and Juanes, 2009). Here we provide the first continuum mathematical model of unstable infiltration in porous media which respects the bounded saturation by construction, therefore overcoming a serious limitation of previous models.

The model is developed based on the phase-field methodology, where liquid saturation is the phase field (Cueto-Felgueroso and Juanes, 2008). We design a new formulation of the free energy of the system and develop a special function of saturation, which we term the capillary pinning function, multiplying the square-gradient term. This function is constructed based on equilibrium considerations in the direction orthogonal to gravity. Our approach leads to a positive pinning function whose structure and properties under fully saturated conditions allow the proposed model, by construction, to honor that water saturations remain bounded.

The proposed continuum model is an extension of the Richards equation with a nonlinear high-order term which introduces a macroscopic surface tension at the wetting front and exhibits a strong link with the capillary pressure. We prove that the proposed model leads to an entropy-increasing evolution for an isolated system. The model reproduces the saturation overshoot at the wetting front and the formation of gravity fingers. Our theoretical analysis shows that the proposed model satisfies the bounded saturation by construction. Our numerical simulations show that the proposed model resolves the pinning behavior at the base of the infiltration front, and confirm the bounded saturation of the proposed continuum model.

References:

Click here to agree

Poster 1 / 768

A coupled wellbore-reservoir model of CO2 flow and heat transfer during a push-pull experiment at Heletz, Israel

Farzad Basirat¹ ; Zhibing Yang² ; Jacob Bensabat³ ; Stanislav Levchenko³ ; Lehua Pan¹ ; Auli Niemi⁵

¹ Department of Earth Sciences, Uppsala University
² Wuhan University
³ Environmental and Water Resources Engineering – EWRE Ltd.
⁴ Earth Sciences Division, Lawrence Berkeley National Laboratory
⁵ Uppsala University

Corresponding Author(s): farzad.basirat@geo.uu.se

To quantify in-situ CO2 residual trapping for CO2 geological storage, dedicated push-pull experiments have been carried out at the Heletz, Israel pilot CO2 injection site. The site is well characterized and instrumented for CO2 injection and sophisticated sampling and monitoring (Niemi et al., 2016) and residual trapping experiments have been carried out during 2016-2017. The objective of the present work is to develop a simulation model capturing the CO2 transport and trapping behavior consistent with the recorded pressure and temperature data at the injection well, with special focus on the coupled wellbore-reservoir flow. For this purpose, the simulation of the CO2 push-pull (injection-withdrawal) experiment is carried out with the numerical simulator T2Well/ECO2N (Pan et al., 2011) to account for the role of wellbore-reservoir coupling. Of particular interest in this work is to accurately model the period when the well is self-producing fluids and to analyze what conditions are causing the observed gas-release behavior. Comparison of numerical model simulations and the measured data suggests that the gas saturation in the reservoir at the onset of the self-release period is only slightly above the residual gas saturation of the formation. In addition, the results indicate that the effective permeability in the reservoir is small enough to be the controlling factor for the gas inflow rate into the wellbore. This detailed modeling of the well self-release behavior allows a more reliable overall estimation of the in-situ residual trapping at the site.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 226

A digital rock workflow to quantify sub-core scale spreading and mixing in reservoir rocks

Author(s): Takeshi Kurotori¹

Co-author(s): Christopher Zahasky ² ; Sayed Alireza Hosseinzadeh Hejazi ¹ ; Sally Benson ² ; Ronny Pini ¹

¹ Imperial College London
² Stanford University
Corresponding Author(s): takeshi.kurotori13@imperial.ac.uk

We report on an extensive investigation of solute mixing and spreading in reservoir rocks, including Bentheimer Sandstone (BS), Ketton Limestone (KL), Edward Brown (EB) carbonate and Indiana Limestone (IL), as well as unconsolidated bead pack (BF) as control material. We observe that the selected rock samples possess distinct strength of subcore-scale heterogeneity and present characteristic features, such as uniform pore structure (BS), a significant degree of microporosity (KL, IL) as well as vuggy porosity (EB). Helium pycnometry, mercury intrusion porosimetry and micro-CT image analysis were applied on small sub-sets (plugs) of each rock samples to provide a distribution of baseline microscopic properties, such as skeletal density, porosity, pore- and grain-size distribution. Unidirectional pulse-tracer tests have been carried out on each rock core over a range of Peclet numbers (Pe = 20–400) and by simultaneously measuring breakthrough curves to provide estimates of the solute longitudinal dispersivity. The unique aspect of this study is that the tracer tests are supplemented by the combination of two imaging techniques: X-ray Computed Tomography (CT) is used to quantify subcore-scale heterogeneities in terms of porosity and permeability contrasts at a spatial resolution of approximately 10 mm³, while Positron Emission Tomography (PET) is applied to image the spatial and temporal evolution of the full tracer plume non-invasively. The latter provides unprecedented insight on the transport mechanisms inside the porous sample at a resolution of a few mm (Figure 1 - image attached). Most significantly, PET imaging enables computing macroscopic measure of mixing as a function time, such as spatial moments, the dilution index and the scalar dissipation rate, which in turn serve as quantitative metrics to compare observations for the different rock samples. Different models have been successfully applied to match the observed breakthrough curves, including the classic Advection-Dispersion Equation, the Multi-Rate Mass Transfer model and their combination within a streamtube framework. The validity of each model was assessed by evaluating its capability to predict the internal tracer concentration profiles measured by PET.

We observe that the effects of macrodispersive spreading can overcome those of local dispersion for heterogeneous rocks (particularly carbonates). In this context, the use of PET in combination with X-ray CT provides significant opportunities to advance our understanding of miscible displacements in consolidated porous media, thus including those involving additional phenomena, such as adsorption, chemical reactions and capillary effects.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 187

A domain decomposition method to couple nonisothermal compositional gas liquid Darcy and free gas flows

Roland Masson¹ ; Nabil Birgle¹ ; Laurent Trety²

¹ University Côte d’Azur, LJAD-CNRS-Inria
² Andra

Corresponding Author(s): roland.masson@unice.fr

A domain decomposition algorithm is introduced to couple non isothermal compositional gas liquid Darcy and free gas flow and transport. At each time step, our algorithm solves iteratively the nonlinear system coupling the nonisothermal compositional Darcy flow in the porous medium, the RANS gas flow in the free-flow domain, and the transport of the species and of energy in the free-flow domain. In order to speed up the convergence of the algorithm, the transmission conditions at
the interface are replaced by Robin type boundary conditions. The Robin coefficients are obtained from a diagonal approximation of the Dirichlet to Neumann operator related to a simplified model in the neighbouring subdomain. The efficiency of our domain decomposition algorithm is assessed on several test cases focusing on the modeling of the mass and energy exchanges at the interface between the geological formation and the ventilation galleries of geological radioactive waste disposal.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 128

A ferroelectric liquid crystal confined in cylindrical nanopores: Reversible smectic layer buckling, enhanced light rotation and extremely fast electro-optically active Goldstone excitations

Mark Busch¹; Andriy Kityk²; Wiktor Piec⁶; Przemyslaw Kula²; Sylwia Calus³; Tommy Hofmann²; Dirk Wallacher³; Martin Steinhart³; Manfred Eich³; Patrick Huber⁴

¹ Hamburg University of Technology

Corresponding Author(s): patrick.huber@tuhh.de

The orientational and translational order of a thermotropic ferroelectric liquid crystal (2MBOCBC) imbibed in self-organized, parallel, cylindrical pores with radii of 10, 15, or 20 nm in anodic aluminium oxide monoliths (AAO) are explored by high-resolution linear and circular optical birefringence as well as neutron diffraction texture analysis. The results are compared to experiments on the bulk system. The native oxidic pore walls do not provide a stable smectogen wall anchoring. By contrast, a polymeric wall grafting enforcing planar molecular anchoring results in a thermal-history independent formation of smectic Chelices and a reversible chevron-like layer buckling. An enhancement of the optical rotatory power by up to one order of magnitude of the confined compared to the bulk liquid crystal is traced to the pretransitional formation of helical structures at the smectic-A-to-smectic-C* transformation. A linear electro-optical birefringence effect evidences collective fluctuations in the molecular tilt vector direction along the confined helical superstructures, i.e. the Goldstone phason excitations typical of the para-to-ferroelectric transition. Their relaxation frequencies increase with the square of the inverse pore radii as characteristic of plane-wave excitations and are two orders of magnitude larger than in the bulk, evidencing an exceptionally fast electro-optical functionality of the liquid-crystalline-AAO nanohybrids.

References:

M. Busch et al., Nanoscale (in press) 2017 DOI: 10.1039/C7NR07273B  Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 607

A field-scale streamline-based simulation of nanoparticle transport in porous media

Bin Wang¹; Yin Feng²; John Beale³; Richard Hughes³; Karsten Thompson³

¹ Louisiana State University
² University of Louisiana at Lafayette
Modeling nanoparticle (NP) transport in porous media is an important research topic in many subsurface engineering applications, such as enhanced oil recovery (EOR), fracture electromagnetic imaging and environmental remediation. An efficient field-scale simulation framework is critical for predicting NP performance and designing subsurface applications. In this work, an efficient streamline-based model is presented to simulate NP transport in field-scale subsurface systems by considering several engineered NP behaviors, such as retention, encapsulation, fluid viscosity change and rock permeability change.

The presented model implements the streamline-based simulation (SLS) approach and operator-splitting (OS) method in NP transport modeling. SLS has been proved to be quite efficient for solving transport in large and heterogeneous systems, where the pressure and velocity field are firstly solved on underlying grids using finite-difference (FD) method. After tracing streamlines, one-dimensional (1D) NP transport is solved independently along each streamline. OS offers the greater flexibility in selecting numerical schemes to solve different governing equations efficiently and accurately. For the NP transport model, explicit FD scheme, implicit FD scheme and adaptive numerical integration are used to solve advection, diffusion and retention terms, respectively.

The presented method is implemented in an in-house streamline-based simulator, it is verified against analytical solutions, a commercial FD reservoir simulator (ECLIPSE) and an academic FD colloid transport code (MNM1D). In the 1D homogeneous case, the effluent breakthrough curves (BTC) of the in-house simulator shows a good agreement with the analytical solution and MNM1D, respectively. In the 2D heterogeneous case, the BTC, cumulative production curve and concentration map of the in-house simulator all matches well with the ECLIPSE solution. In addition, a synthetic 3D engineering design case, NP capsule gelation flooding, is performed to investigate the effect of displacing fluid and NP properties on displaced fluid production. Results show that the NP retention capacity and displacing fluid viscosity are the two dominant factors affecting the flooding performances. The CPU time of the synthetic case are also reported, where 8-30 minutes are required to simulate a 7-19 species system in a laptop.

References:

Acknowledgements

This work was supported by the Advanced Energy Consortium (http://www.beg.utexas.edu/aec/) with BHP Billiton, Department of Energy, ExxonMobil, Repsol, Shell, and Total as members.


Acceptance of Terms and Conditions:

Click here to agree
**Poster 4 / 241**

**A fractal study on effective thermal conductivity of porous media**

Jianchao Cai¹ ; Xuan Qin¹ ; Wei Wei¹ ; Yuxuan Xia¹

¹ China University of Geosciences (Wuhan)

**Corresponding Author(s): caijc@cug.edu.cn**

Thermal conduction in natural porous media has been deeply paid attention in science and engineering, for example, exploiting and utilizing the geothermal energy, determining the heat flow in hydrothermal systems, obtaining the information about the past climate, modelling the hydrocarbon formation processes and investigating the potential nuclear wastes, etc. The thermal conductivity plays an important role in these fields. Since thermal conductivity is usually difficult to measure, a theoretical model of thermal conductivity inferred from other physical properties is needed. As we all know, the thermal conductivity is strongly influenced by the microstructure features of porous media. In this work, based on the fractal characteristics of the grains, a theoretical model of effective thermal conductivity is proposed for saturated and unsaturated porous media. It is found that the proposed effective thermal conductivity solution is a function of geometrical parameters of porous media, such as the porosity, fractal dimension of granular matrix and the thermal conductivity of the grains and pore fluid. The model predictions are compared with existing experimental data and the results show that they are in good agreement with existing experimental data. The proposed model may provide a better understanding of the physical mechanisms of thermal transfer in porous media than conventional models.

**References:**


**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 10-E / 507**

**A groundwater flow model: Flow behavior through anisotropic granular porous media**

**Author(s):** Andres Abad Gonzalez ¹

**Co-author(s):** Pavan Veluvali ¹ ; Aron Kneer ¹ ; Andreas Reiter ² ; Britta Nestler ³ ; Michael Selzer ¹ ; Patrick Altschuh ³

¹ Karlsruhe University of Applied Sciences - Institute of Digital Materials Science
² Karlsruhe University of Applied Sciences - Institute of Digital Materials Science
³ Karlsruhe Institute of Technology - Institute of Applied Materials

**Corresponding Author(s):** andres.abad_gonzalez@hs-karlsruhe.de

The flow behavior through porous media is yet to be fully understood. The comprehension of the fundamental physical mechanisms and of the dynamics can significantly help the development of many applications in the engineering field.
A porous system can be formed by natural as well as by artificial processes, and is mostly described by granular media, compacted under external forces. The pore size and pore size variation are strongly dependent on the grain topology and size distribution. Most of the naturally formed porous media exhibit an anisotropic behavior, an example of which are soil formations created by sedimentation processes over long periods of time.

In the case of groundwater remediation, the flow is superimposed by a forced convection, which is induced by recirculation wells with integrated pumps. The main idea of groundwater recirculation is to enforce vertical flow paths through the ground, and to increase the radius of influence of the remediation process, which is determined by the soil resistance against the flow. The permeability and conductivity of the soil layers dictate the flow behavior in various directions. The knowledge of this operating range and of the correlations between influencing quantities, is essential for the layout of groundwater remediation technologies.

For an accurate description of the flow behavior through soil layers, several geometric parameters which characterize the anisotropic nature of the granular media, must be considered. Therefore, the generation of a realistic 3D topology of the soil formation is fundamental. Within this work, an extensive characterization of the shape complexity, the surface roughness, and the size distribution of granular structures in natural soil formations, is performed. Furthermore, a study of the dense nature of the grain packing is conducted. The results are used to generate realistic soil models, constituted by 3D granular structures with defined size distributions, by specialized filling algorithms. Digital models, based on experimental data, are used to set up a flow model for simulation studies. The main objective is to determine the anisotropic flow resistance as a 3D tensor, which can be used as an input parameter for the construction of macroscopic groundwater flow models, with much less computational effort. Furthermore, the simulation studies provide relevant information concerning contaminant mobilization, the effect of forced convection, and the radius of influence under different operation conditions and soil compositions. An additional benefit of the computational studies is the possibility to characterize not only natural soil formations but also almost any entangled granular porous media by their hydraulic properties.

Being able to obtain a 3D hydraulic conductivity tensor from realistic underground soil structure topologies is a big step forward towards the understanding of underground water flow.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8·G / 227

A linearly stable, implicit WENO scheme applied to two-phase flow in porous media

Author(s): Todd Arbogast

Co-author(s): Chieh-Sen Huang ; Xikai Zhao

1 University of Texas at Austin
2 National Sun Yat-sen University
3 University of Texas

Corresponding Author(s): arbogast@ices.utexas.edu

We present a general implicit weighted essentially non-oscillatory (iWENO) method for solving advection-diffusion equations that is locally conservative and third order accurate, simple to implement, and allows general computational meshes. The scheme is quite robust, since it is unconditionally stable for smooth solutions to linear problems in 1D. The scheme requires only two unknowns per computational mesh element, independent of the spatial dimension, so it is maximizes the mesh resolution. This is important physically, so that natural heterogeneities in porous materials can be resolved, which alone can allow fine features in the medium and/or the solution to be well resolved.
It is also important computationally for modern high performance computers, which are memory bandwidth limited, since the scheme emphasizes many local computations using a small amount of data. Application to two-phase flow in porous media will be presented.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-C / 923

A multiscale flux basis for mortar mixed discretizations of reduced fracture models

Elyes Ahmed¹; Alessio Fumagalli²

¹ University of Bergen

Corresponding Author(s): elyes.ahmed@uib.no

We are concerned with the application of nonoverlapping domain decomposition methods on reduced fracture models. We provide for this problem a new DD algorithm in which the global problem is reduced to a mortar problem posed on the fractures that is solved by an iterative solver. Classical iterative methods are based on the CG or optimized Schwarz waveform methods which require solving one local Dirichlet or Robin problem on each subdomain per interface iteration. Increasing the number of fractures and refining the grids both lead to an increase in the number of iterations and the number of subdomain solves. One way to eliminate this dependency between the total number of subdomain solves and the fractures solves is to use multiscale basis functions. Precisely, the proposed algorithm involves precomputing the flux or velocity actions from the subdomains, called multiscale flux basis, associated with each mortar degree of freedom on every subdomain. This requires a fixed number of subdomain solves. Then, the subdomain solves required at each interface iteration are replaced by linear combinations of the precomputed multiscale flux basis functions. We test our algorithm on various test cases for two types of fractures, fractures which have a permeability higher than that in the surrounding medium and those in which the permeability is lower than that in the surrounding medium.

References:


Click here to agree

Parallel 8-H / 498

A multiscale method with Robin boundary conditions for the porous media equations

Rafael Trevisanuto Guiraldello¹; Roberto Federico Ausas¹; Fabricio Sousa²; Felipe Pereira³; Gustavo Carlos Buscaglia³

¹ University of São Paulo - São Carlos
The design of accurate multiscale domain decomposition methods for channelized, high-contrast porous media remains as an important challenge in typical problems posed by the oil industry. Here we investigate an improved version of the recently proposed Multiscale Robin Coupled method (MRCM). This method ensures weak continuity of both normal fluxes and pressure through the imposition of Robin-type boundary conditions at the skeleton of the domain decomposition where the interface spaces $\mathcal{P}$ and $\mathcal{U}$ for the pressure and fluxes, respectively, can be chosen independently. The MRCM can be seen as a generalization of two well-know multiscale procedures, the Multiscale Mixed Mortar Finite Element method (MMMFEM) and the Multiscale Hybrid Method (MHM). In this work, we compare the accuracy of the above mentioned multiscale procedures given a fixed computational cost for polynomial and informed spaces. Our results illustrate how one can take advantage of the built in flexibility of the MRCM to produce more accurate results when compared to the MMMFEM and MHM.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-E / 671

A multiscale two-equation reaction-diffusion porous media model of gas exchange in apple fruit

Siem Janssen1 ; Susana Zorrilla2 ; Bart Nicolaï3 ; Pieter Verboven4

1 KU Leuven - University of Leuven, division BIOSYST-MeBioS
2 INTEC (CONICET - Universidad Nacional del Litoral)
3 KU Leuven - University of Leuven, Division BIOSYST-MeBioS; VCBT – Flanders Centre of Postharvest Technology
4 KU Leuven - University of Leuven, Division BIOSYST-MeBioS

Corresponding Author(s): pieter.verboven@kuleuven.be

Pome fruit such as apple are harvested mature but unripe, stored at low temperature (typically -1.0 to 3°C) in combination with a reduced O₂ and increased CO₂ partial pressure in so-called controlled Atmosphere (CA) storage. This is done to delay climacteric ripening, and, hence, extend their storage life. The optimal storage gas composition is critical, as too low O₂ levels in combination with too high CO₂ levels may induce fermentation in the fruit. This causes off-flavours (e.g., ethanol) and storage disorders (e.g., flesh browning). Using a materials engineering approach fruit tissue is considered a microporous structure consisting of parenchyma cells with air spaces in between. Based on in silico experiments we have shown that large concentration gradients and anoxic zones may indeed occur in pome fruit. Porosity and connectivity of the intercellular spaces have been shown to affect O₂ and CO₂ transport to a large extent. We previously developed a homogenized reaction-diffusion model to study gas exchange of intact fruit at the macroscale level, which was based on the assumption of gas-liquid equilibrium in the cellular material, of which the material properties were determined from microscale simulations in a multiscale approach. Here we explore if the equilibrium assumption holds by developing and solving a two-equation model at the macroscale, which
distinguishes transport in gas and liquid phase separately with mass transfer between the phases. To identify the model parameters of the macroscale two-equation model, a microscale model was developed. To this end, the 3-D tissue geometry of apple (cv. Jonagold) tissue obtained from X-ray microtomography was processed to calculate geometrical parameters (porosity and specific surface of the interface). The microstructure was also input for an adapted voxel based finite volume code that calculated effective gas transport properties of the two phases of the apple tissue separately. The two-equation model was then solved using finite elements on the reconstructed geometry of apple fruit and the resulting internal gas profiles were compared to those obtained from the one-equation equilibrium model. Under the same conditions and values of interphase permeability and respiration rates previously used in our analyses, the two-equation model did not have significant differences with the one-equation model, which is more than 5 times faster to solve. We also explored if realistic value ranges of permeability and reaction rates exist for which the one-equation would not be valid and the two-equation solution would be required.

References:


Click here to agree

Parallel 8-H / 442

A new coupled approach for numerically solving convection-diffusion problems with discontinuous capillary pressure

Arthur Santo¹ ; Eduardo Abreu²

¹ University of Campinas
² University of Campinas, Sao Paulo, Brazil

Corresponding Author(s): arthurm@ime.unicamp.br

In this work, we show an alternative way of handling the spatially discontinuous capillary pressure models in two-phase flow in porous media. This topic is very challenging and has also been studied theoretically and numerically in recent works [1,2,3]. We propose a new numerical formulation, by combining mixed hybrid finite element and finite volume discretization strategies along with novel coupling conditions at interfaces for numerically solving convection-diffusion problems
with gravity and diffusive discontinuous capillary pressure. The novelties are twofold: 1) a reinterpretation of the Robin interface conditions between elements to accommodate the nontrivial effects of heterogeneities in capillary pressure and 2) the use of a conservative finite volume framework for approximation of the first-order hyperbolic flux in a robust fashion as a source term in the fully coupled formulation to preserve the delicate nonlinear balance with the diffusive operator. By following [4], we also present preliminary results and further directions that relates the new approach to multiscale formulations for porous media transport problems in the presence of high contrast geological properties.

References:


Click here to agree

Poster 3 / 1101

A new dynamic permeability model of coal considering pore compressibility, matrix shrinkage and pulverized coal output and blockage

Author(s): Juntai Shi

Co-author(s): Shan Wang ¹; Chenhong Hou ¹; Kun Feng ²; Kamy Sepehrnoori ³

¹ State Key Laboratory of Petroleum Resources and Prospecting in China University of Petroleum at Beijing
² PetroChina Coalbed Methane Company Limited
³ The University of Texas at Austin

Corresponding Author(s): juntai.shi@gmail.com

As an unconventional gas resource, coalbed methane (CBM) reservoir has unique flow mechanism and production scheme compared with conventional and other unconventional gas reservoirs. The permeability of coal cleats system varies with the production of water and gas, in order to accurately forecast gas productivity, the dynamic permeability model should be investigated first before establishing gas production model of CBM wells. At present, many investigators have proposed some dynamic permeability models of coal correlating to pressure during CBM production process. However, few studies consider pore compressibility, coal matrix shrinkage, pulverized coal output and blockage in the model at the same time.

In this paper, firstly, the porosity model is established based on stress sensitivity effect and matrix shrinkage effect separately. Secondly, the variation mechanism of the porosity with pressure resulted from pulverized coal output and blockage is investigated and the corresponding correlation is built up by fitting the current experimental data and pulverized coal output data from actual CBM wells. Thirdly, coupling stress sensitivity effect, matrix shrinkage effect and pulverized coal output and blockage effect together, the united porosity model with pressure is proposed, and then on the basis of PM model, the dynamic permeability model considering these three effects is derived. Finally, the model is validated by data from literatures, then factors influencing on permeability is analyzed, and the rational dewatering schedules are suggested for CBM reservoirs with different ranks, gas contents and permeabilities.

Good agreements between permeabilities from literatures and those calculated by the proposed model are obtained, indicating that the proposed dynamic model of coal cleat system is rational and accurate to apply in the establishment process of water and gas productivity model for CBM wells.
Results show that: if only considering stress sensitivity effect, the permeability of coal cleat system decreases sharply first and then smoothly with decreasing pressure; if only considering coal matrix shrinkage effect, the permeability remains constant before desorption but increases with decreasing pressure after desorption; if only considering pulverized coal output and blockage effect, the permeability remains constant at higher pressure but increases slightly because of pulverized coal output and then decreases gradually with pressure because of pulverized coal blockage; if considering these three effects simultaneously, the permeability decreases first and then might decrease or increase at the late time with decreasing pressure. At the dewatering stage, the bottom hole flowing pressure should be controlled near the critical pressure with maximum pulverized coal output, while, at gas production stage of CBM wells, the difference between average pressure and bottom hole flowing pressure should be controlled at some value with maximum permeability of coal cleat system.

Because the proposed dynamic permeability model considers three different mechanisms of fluid through coal cleats simultaneously, the permeability variation with pressure and the corresponding productivity of CBM wells can be accurately forecasted. The dewatering and production schedules for different types of CBM reservoirs can also be determined using this dynamic permeability model of coal.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-H / 721

A new iterative downscaling procedure for multiscale methods in porous media flows

Franciane Rocha¹; Fabricio Sousa¹; Rafael Trevisanuto Guiraldd³; Felipe Pereira³; Roberto Federico Auras³; Gustavo Carlos Buscaglia²

¹ University of Sao Paulo
² University of Sao Paulo - Sao Carlos
³ Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA

Corresponding Author(s): fsimeoni@icmc.usp.br

Non-overlapping domain decomposition multiscale methods have been successfully applied to flows in porous media. Such remarkable class of methods seek to decompose the domain of the porous media flow equations in non-overlapping subdomains, solving smaller local problems in parallel, and one global interface problem, instead of a large coupled one. Usually the interface problem enforces the compatibility conditions — continuity of pressures and normal fluxes — across subdomain interfaces. In multiscale methods, these conditions are enforced at different length scales, originating different methods. Examples are the MMMFEM [1] (Multiscale Mixed Mortar Finite Element Method), that prioritize pressure continuity at fine scales and weak flux continuity; the MHM [2] (Multiscale Hybrid-Mixed Method), that enforces continuity of normal fluxes at fine scales and weak pressure continuity; the MuMM [3] (Multiscale Mixed Method) that enforces weak continuity of both pressure and normal fluxes through Robin-type boundary conditions. Recently, the MRCM [4] (Multiscale Robin Coupled Method) that generalizes the aforementioned methods in one single variational formulation has been introduced.

It is well known that enforcing continuity only at larger scales creates a discrepancy in the continuity (of pressure or normal fluxes, or both) in fine scales, so that a downscaling is required to keep the resulting velocity fields conservative.

We propose a new iterative procedure based on alternating domains with minimum overlapping to perform downscaling of the computed normal fluxes, resulting in new conservative velocity fields. We studied the applicability and efficiency of this new method when applied to multiphase flow problems using the MRCM, as compared to existing techniques, illustrating the advantages of our new procedure.
A new method based on high-resolution imaging of pore space for rock typing

Author(s): Yongjie MA¹ ; Xin WANG¹
Co-author(s): Qi ZHANG¹ ; Fengli YANG¹ ; Ye XU² ; Jingsheng MA²

¹ Institute of Oceanographic Instrumentation, Shandong Academy of Sciences
² Beihang University

Rock typing is an essential step in reservoir characterization and geological model building for reservoir simulation. Conventionally porosity, permeability and capillary pressure data of coring core samples are used to divide rock types. With developing of high-resolution imaging equipment, micro-structure parameters are able to be quantified and wildly used in the research of reservoir characterization. Based on high-resolution imaging technology, we proposed a new method that quantifies pore space structure of different rock types with different micro-structures. Firstly, we apply Minkowski functions to get the distribution of connectivity at different pore diameters, tortuosity and specific surface area etc.; secondly, we use pore network model and Lattice-Boltzmann model to simulate the conductivity of the 3D image of rocks; Then we compared conductivities for a serious of rock samples, and got the correlation between conductivity and micro-/macro- parameters. We also got the conductivity’s sensitivity of the parameters. We believe they all have positive effects on rock typing study.

References:

Acceptance of Terms and Conditions:

Click here to agree
Corresponding Author(s): katharina.heck@iws.uni-stuttgart.de

We present a general model concept and a flexible software framework for the description of plant-scale soil-root interaction processes including the essential fluid mechanical processes in the vadose zone. The model is developed in the framework of non-isothermal, multi-phase, multi-component flow and transport in porous media. The software is an extension of the open-source porous media flow and transport simulator ‘dmux’ to embedded mixed-dimensional coupled schemes. Our coupling concept allows us to describe all processes in a strongly coupled form and adapt the complexity of the governing equations in favor of either accuracy or computational efficiency. We present the necessary numerical tools to solve the arising strongly coupled non-linear PDE systems with a locally mass conservative numerical scheme even in the context of evolving root architectures. We demonstrate the model concept and its features discussing a virtual hydraulic lift experiment including evaporation, root tracer uptake on a locally refined grid, the simultaneous simulation of root growth and root water uptake, and an irrigation scenario comparing different models for flow in unsaturated soil. We analyze the impact of evaporation from soil on the soil water distribution around a single plant’s root system. Further, we show that locally refined grids around the root system increase computational efficiency while maintaining accuracy. Finally, we demonstrate that the assumptions behind Richards equation may be violated under certain conditions.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-G / 286

A nonlinear asymptotic model for the inertial flow at the interface of a permeable medium

Benoit Goyeau¹ ; Philippe Angot² ; J. Alberto Ochoa-Tapia³

¹ Ecole Centrale-Supélec, Université Paris-Saclay, EM2C, CNRS UPR-288,
² Aix-Marseille Université, Institut de Mathématiques de Marseille, CNRS UMR-7373, Centrale Marseille
³ Universidad Autonoma Metropolitana-Iztapalapa

Corresponding Author(s): benoit.goyeau@centralesupelec.fr

A two- or three-dimensional nonlinear model for the inertial incompressible viscous fluid flow at a fluid-porous interface is proposed [1]. The interfacial region between the pure fluid and the homogeneous porous region is viewed as a thin transition porous layer characterized by evolving heterogeneities [2-4]. An asymptotic analysis [5] is applied to the homogenized Navier-Stokes equation giving rise to nonlinear jump conditions for the momentum transport with inertia at the equivalent dividing interface. These jump conditions involve slip and friction coefficients whose dependence on the porosity are analyzed. In addition, we show that the global work of the inertial forces in the fluid and porous regions has always a positive contribution at the interface to the dissipation of kinetic energy inside the whole system. To our knowledge, this innovative asymptotic model is the first multi-dimensional nonlinear model proposed in the literature for the inertial flow. Moreover, it clearly opens new perspectives to study turbulent flows at the fluid-porous interface.

References:

Poster 3 / 279

A novel pore structure reconstruction procedure facilitating simulative analysis of multiphase displacement processes in porous media

Dongxing Du\(^1\); Guolong Sun\(^1\); Yingge Li\(^1\); Lichen Zheng\(^1\); Chengcheng Wang\(^1\)

\(^1\) Qingdao University of Science and Technology

Corresponding Author(s): du-dongxing@163.com

With the increasing demand for enhancing production of oil and gas all over the world, improving oil recovery technologies aiming at developing low permeable and tight oil reservoirs are becoming the focus of current research. To help understanding the mechanism of multiphase displacement in underground reservoir, the microcosmic characterization of porous media must be explored. In recent years, Digital rock physics (DRP) technology for simulative analysis of rock physical properties based on extracted CT scanning images plays more and more important roles in geosciences, soil science, petroleum engineering and many other fields.

In this paper, A novel procedure is proposed for accurate reconstruction the 3-D pore internal structures, based on which the pore volume is successfully meshed for further detailed numerical investigations of the multiphase displacement process in porous media. The first step is to determine the REV of the studied rock after processing the all the CT images with the software of ImageJ®, with which the image noise reduction, threshold segmentation and binarize processes are carried out. The second step is to employ Matlab® software to transform the binary black and white series of rock images into a digital 3-D matrix consists of 0 and 1. Then reconstruction of the pore void volume is performed through employing the software of ProE®, which could supply the compatible format for the fluid dynamics analysis software of Fluent®. Single phase and two-phase displacement processes are numerically investigated with the software of Fluent® in the reconstructed pore structures. Numerically obtained gas permeability is 2.02D, which reasonably lies in the region of 1.2-3D of the Bentheimer core samples. It is concluded the proposed novel rock internal structure reconstruction procedure can ensure the simplicity and accuracy on predicting the multiphase transport characteristics in porous media.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-G / 584

A novel transient diffuse source algorithm for multiscale simulation in porous media

Krishna Nunna\(^1\); Michael King\(^1\)

\(^1\) Texas A&M University

Corresponding Author(s): nkchaitanya@tamu.edu

Fluid flow in porous media occurs on varied scales from pore to reservoir, where the fine scale heterogeneity may have a significant impact on large scale fluid flow. Resolving all pertinent scales in modeling and flow simulation is an arduous task limited by the availability of data and computational
resources. Therefore, it is customary to use an upscaling procedure, in which the fine scale reservoir properties are represented on the coarse scale by some kind of averaging procedure. Existing local upscaling methods rely on steady state incompressible flow, which fail to capture transient multiscale effects. Particularly, they cannot preserve the dynamic connectivity while coarsening between multiple scales. This results in overly homogenized simulation models with systematically biased results. This same bias can be observed in multiscale flow simulation where large scale changes in pressure are resolved on the coarse scale, and multiphase fluid transport simulation is performed on the fine scale using a subgrid velocity field generated from the coarse problem. This precludes the need to upscale saturations and relative permeability which are highly non-linear and strongly dependent upon flow history. The current work combines the upscaling of pressure with multiscale multiphase simulation to generate high resolution velocity fields that capture the subgrid heterogeneity, fluid compressibility, and multiphase flow.

The upscaling step draws upon its similarity to pressure transient well testing concepts to set up local flow problems. Instead of a wellbore, each local problem is performed from a coarse cell face. This enables us to distinguish between well-connected and weakly connected pays while upscaling. This approach is similar to the multiscale mixed finite element literature where we have a basis function for a coarse face. After upscaling, superposition principle allows us to downscale the coarse flow, generating the fine scale velocity field. Finally, the transport problem is solved on the fine scale giving fluid saturations.

The proposed method is validated on the high contrast SPE10 synthetic model with over 8 orders magnitude variance in permeability, and demonstrated on a full field tight gas reservoir model.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-B / 485

A numerical model for reactive transport coupled with microbial growth on Darcy scale

Author(s): Birger Hagemann ¹

Co-author(s): Mikhail Panfilov ²; Leonhard Gänzer ¹

¹ Clausthal University of Technology
² Université de Lorraine

Corresponding Author(s): birger.hagemann@tu-clausthal.de

The injection of substrates, e.g. hydrogen with the purpose of energy storage, into subsurface structures could stimulate the growth of all present microbial species which are able to use this substrate for their metabolism. The linkage between transport, the growth of microorganisms, substrate availability and biodegradation results in a strongly coupled dynamic system. The difficulty in the development of a general model is the inclusion of processes which appear on different length and time scales. In this work, a flexible numerical model was developed which uses effective representations of the processes on Darcy scale. The mass exchange between two phases (gas and water) is treated instantaneously by using an equilibrium law. Multiple metabolic reactions can be included kinetically by defining the stoichiometry and kinetic coefficients. Different mathematical models can be selected to describe the substrate-limited microbial growth. Microorganisms can be considered as an immobile biofilm or as partially mobile within the water phase. The time-like appearance of usual growth models and the strong coupling to the reactive transport equations results in a very stiff equation system. The numerical instability was overcome by a proper adaptive time step selection and a check for the physical possibility of each solution before it is continued to the next one. Example simulations are shown for a near wellbore and a field scale study of an underground hydrogen storage.
Parallel 10-F / 666

A numerical modeling approach for capillary effects in systems with changing porosity

Peter Johnson¹ ; Philip Stauffer¹ ; George Zyvoloski¹

¹ Los Alamos National Laboratory

Corresponding Author(s): pjjohnson@lanl.gov

Most commonly used numerical models of unsaturated porous media flow use a single capillary retention function which is specified at the start of the model run and alters capillary pressure only as a function of saturation. However, changes in porosity are common in geologic and industrial applications across a wide range of time scales. Consequently, numerical models of unsaturated media flow in these systems may become inaccurate over the course of a model run. In extreme cases, clearly unphysical results can occur, such as liquid water suspended in newly-created void spaces. In less extreme cases, the single retention function has a tendency to balance saturation to the same value throughout the region to which the function is applied, independent of any changes in the porous medium. Water in these cases tends to be drawn out of low-porosity regions into high-porosity areas to achieve this balance, but low-porosity porous media should generally be harder to drain and retain a higher saturation. Such inaccuracies tend to produce counterintuitive results, especially with volumetric water content, and can be compounded in scenarios where porosity changes are driven in part by that volumetric water content. One example where this problem may arise is in numerical modeling of high-temperature sources in salt, where brine/vapor interactions and fluid migration causes porosity changes in the salt via dissolution and precipitation.

To address these issues, we have developed new formulations for the retention function in which residual saturation and maximum capillary pressures are dynamically changed throughout the simulation as local porosity changes. The new functions are applied in the porous flow simulator Finite Element Heat and Mass (https://femn.lanl.gov). In this approach, at a given saturation, capillary forces weaken as node porosity increases, and strengthen as porosity decreases. This approach eliminates the suspended water problem and increases the retention of water in low-porosity nodes. In salt test cases, model outputs are more intuitively reasonable and show strong differences from the initial-only retention curve cases, with dramatic changes in volumetric water content and a reduction in the severity of dissolution effects.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 672

A pore-scale study of viscoelastic surfactant flow through porous media

Brayan F. Garcia¹ ; Soheil Sarají² ; Maysam Mousaviraad ²

¹ University of Wyoming
² University of Wyoming
Corresponding Author(s): bgarcia6@uwyo.edu

The interest in viscoelastic surfactant solutions (VES) as enhanced oil recovery fluids has been increasing in recent years, due to their practical advantages over polymeric solutions. However, during their flow inside the porous medium, complex geometries (such as throats that connect pores) might cause high shear-extensional components, affecting the flow behavior, and therefore the performance of these systems. For that reason, it is important to understand the rheology of these systems and the relationship with different parameters/conditions such as geometries, temperature, flow rates, and concentrations. The aim of this work is to employ an interactive experimental/numerical paradigm where: 1) experimental data are obtained and used in the process of developing the computational model; 2) systematic simulations are designed and carried out to map the rheological response; 3) the simulation data will be used to improve and/or fill the gap in the empirical correlations used in experiments, as well to guide the design of the next round of experimental matrix; and 4) the improved experimental data are analyzed to select a final set of critical conditions, for which the computational model is improved.

We present a comprehensive and systematic experimental-modeling study on pore-scale rheology of three different viscoelastic solutions in a converging-diverging micro-channel. We evaluated the effects of salt/surfactant concentrations, elevated temperatures (up to 65 °C), and flow rates (100-1000 μL/min). We used an extensional Viscometer-Rheometer On a Chip (e-VROC) for these measurements. This system comprises a hyperbolic contraction channel and micro-electro-mechanical systems technology for accurate pressure measurements along the channel. We consider non-ionic, zwitterionic/anionic, and cationic surfactant solutions composed of commercial Aromox APA-TW plus calcium chloride (APA-TW + CaCl2) N-tetradecyl-N,N-dimethyl-3-ammonio-1-propanesulfonate plus sodium dodecyl sulfate and sodium chloride (TPDS + SDS + NaCl), and cetymtrimethylammonium bromide plus sodium salicylate (CTAB + NaSal). A complete analysis of concentrations, temperatures and flow rate effects on extensional rheology is described, providing an extensive results and remarkable highlights of the effects of different parameters on extensional flow behavior of VES.

Computational Fluids Dynamics (CFD) methods will be used for modeling and simulations of the viscoelastic solutions. In the current step, we use the Navier-Stokes equations for an incompressible and isothermal single-phase flow in the two-dimensional micro-channel geometry. In the next steps, additional complexities, physical and geometrical, will be included in the computational model, one at a time, to simulate and study larger patterns such as multiple contraction-expansion geometries in serial configurations, interconnected flow paths and cross-flow, under different flow velocities. Consequently, the numerical results will allow us to design specific experiments using micro-PIV technique that shall expand our understanding on flow behavior of viscoelastic fluids in large patterns of pores and throats extracted from real images of porous rocks. The PIV measurements will also provide flow field data that can be used for comparison with the computational results. In the final step, we intend to perform advanced two-phase experiments on micro-PIV devices and geometries extracted from real porous medium to monitor oil displacement at the microscopic scale.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-G / 126

A posteriori error estimates, stopping criteria, and adaptivity for a two phase flow with exchange between phases as a nonlinear complementarity problem in porous media

Author(s): Jad Dabaghi

Co-author(s): Martin Vohralik \(^1\); Vincent Martin \(^2\); Ibtihel Ben Gharbia \(^3\)

\(^1\) Inria Paris
2 UTC Compiègne
3 IFPEN

**Corresponding Author(s):** jad.dabaghi@inria.fr

In this work we develop an a posteriori-steered algorithm for a two phase compositional flow with exchange of components between the phases in porous media. The discretization of our model is based on a backward Euler scheme in time and a finite volume scheme in space. The phase transition is treated introducing a formulation based on Henry’s law. The resulting nonlinear system is solved via an inexact semi-smooth Newton method. The key ingredient for the a posteriori analysis are the discretization, linearization, and algebraic flux reconstructions allowing to devise estimators for each error component. These enable to formulate criteria for stopping the iterative algebraic solver and the iterative linearization solver whenever the corresponding error components do not affect significantly the overall error. Numerical experiments are performed using the semi-smooth Newton-min algorithm as well as the Fischer–Burmeister algorithm and the GMRES iterative linear solver to show the efficiency of the method.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Poster 2 / 698**

**A random connection model for pore network modeling**

**Author(s):** Ana T. Mendoza-Rosas¹

**Co-author(s):** Martin A. Díaz-Viera¹ ; Edgar G. Martínez-Mendoza³

¹ CONACYT-Centro de Ingeniería y Desarrollo Industrial

² INSTITUTO MEXICANO DEL PETROLEO

³ Universidad Nacional Autónoma de México

**Corresponding Author(s):** ana.mendoza@cidesi.edu.mx

Pore network models have been applied for predicting petrophysical properties at pore scale. From a geometry point of view, basically a pore network and pore and throat size distributions are required for pore network modeling. Although different pore network models have been constructed using data extracted mainly from images, it is not always possible to count on the necessary information, and working with a unique extracted network could generate non-representative results. Therefore, a statistical analysis of the data offers the advantage of generating different realizations of the network and its geometry. Building statistically representative networks require analysis of the image to extract size distributions of pores, throats and their connectivity. The last is relevant for percolation properties of the pore system.

In this work a random connection model (RCM) for network modeling is proposed. In a random connection model the critical density is a connection function g. A connection function defined as g: Rd→ [0, 1] is chosen, where a pair of points (x,y) are connected with probability g(|x - y|), independently of all other pairs of points, here | | denotes Euclidean distance in Rd. In general, if unbounded connected components arise, we say that percolation occurs. The RCM is applied to a case of study for pore network modeling of a carbonate rock sample. In particular, from multiple realizations of the RCM the effect on fluid flow properties is investigated.

**References:**


Poster 3 / 91

A reconstruction method for 3D porous media based on a 3D training image using multiple-point statistics and multiple-grid templates

Author(s): Yuqi Wu

Co-author(s): Chengyan Lin; Lihu Ren; Muhammad Jawad Munawar

1 School of Geosciences, China University of Petroleum (East China)

Corresponding Author(s): wuyuqi150348@163.com

At present, many methods of porous media modeling have been proposed. Among them, the multiple-point statistics (MPS) method has a unique advantage in reconstructing 3D digital rock in that it can characterize long-range connectivity of pore space. The Single Normal Equation Simulation (SNESIM) is one of most commonly used algorithms of MPS. In the SNESIM algorithm, the selection of training image is critical because it contains the basic pore structure patterns. In the previous reconstruction of 3D porous media using SNESIM, a 2D slice was usually employed as the training image. However, it is difficult for a 2D slice to contain complex 3D pore space geometry and topology patterns. In this paper, a 3D training image are used in order to supply the more real heterogeneity of pore space. On the other hand, the multi-grid search template is applied for the purpose of capturing the pore structures of different scales and speeding up the reconstruction process. The Berea sandstone is taken as the test example, 3D porous media of Berea sandstone were reconstructed. The two-point correlation function, pore network structure parameters, absolute permeability, flow velocity and the pressure fields are applied as the evaluation indexes to test the accuracy of the reconstructed models. The comparison result shows that reconstructed models are good agreement with the real model obtained by X-ray computed tomography scanning in the pore throat geometry and topology and transport property, which validates the reliability of the proposed method.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 196

A reduced-order model to assist real-time predictions of gas transport in unsaturated fractured media

John Philip Ortiz; Dylan Robert Harp; Philip H Stauffer

1 Los Alamos National Laboratory, Computational Earth Science
2 Los Alamos National Laboratory, Computational Earth Science

Corresponding Author(s): jportiz@lanl.gov

Gas transport in unsaturated fractured media plays an important role in applications such as shallow CO2 leakage from carbon sequestration sites, methane leaks from oil and gas operations, and remediation of volatile contaminant plumes. Driven primarily by barometric pumping, the time scale of relevant gas transport can vary from months or years to the order of days depending on a variety of hydrogeologic parameters, including: rock type, fracture aperture, matrix permeability, porosity, and saturation. It is very difficult to use computationally expensive numerical simulations to make real-time predictions of gas transport when parameter uncertainty is high and/or there is potential
for rapid transport. We propose a reduced-order model (ROM) of gas transport in fractured media as a means of reducing computational complexity and allowing quicker approximations of migration time scales to assist real-time decision-making as it concerns gas transport. We build our ROM using relationships from a parameter sensitivity study of a two-dimensional single-fracture numerical flow and transport model simulated using PFLOTRAN and FEHM codes. Our modeled flow results are benchmarked where appropriate by a corresponding analytical solution for the subsurface pressure response from a harmonically varying barometric pressure fluctuation at the surface. This ROM can aid in bracketing real-time estimates of gas transport and has the potential to be generalized to more complex three-dimensional and discrete fracture networks.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-C / 63

A stress-driven DFN model to account for fracture network geometrical complexity

Etienne Lavoine¹; Philippe Davy²; Caroline Darcel¹; Raymond Munier³

¹ Itasca Consultants SAS
² Géosciences Rennes UMR CNRS 6118, Rennes, France
³ Svensk Kärnbränslehantering AB

Corresponding Author(s): etienne.lavoine@univ-rennes1.fr

Discrete Fracture Network (DFN) models are the geometrical basis for flow simulation of poro-fractured media in many industrial projects such as deep waste disposal, hydrogeology or petroleum resources. Because the spatial organization of fractures may control the hydrological and mechanical behavior of the fractured rock mass, the geometrical complexity of the network is a key point of the modeling workflow. This complexity is beyond the reach of purely stochastic DFN models, referred as “Poisson models”, which neglect the potential importance of fracture-to-fracture interactions, and the consequent modifications of the spatial organization and connectivity of the network. Fracture network development is a complex feedback-loop process between the propagation of fractures and the emergence of new ones. Using genetic models of fracture networks to replace the lack of field information may be a solution for realism. Recent papers (Davy et al., 2010; Davy et al., 2013) have proposed a genetic model of DFN, called "UFM model", using simplified fracturing-relevant rules for nucleation, growth and arrest of fractures. With simple kinematic rules that mimic the main mechanical processes, the model produces fracture size distributions and fracture intersections that are consistent with observations. Our objective is to improve the model by explicitly considering the control of local stresses in both nucleation and fracture growth. This has the advantage of linking the geometry and topology of fracture networks with the assumed conditions of their formation. We introduce a stress-driven nucleation in the timewise process of this kinematic model to study the correlations between nucleation, growth and existing fracture patterns. The method calculates the stress field generated by existing fractures and the allegedly known remote stress as an input for a Monte-Carlo sampling of nuclei centers at each time step. The orientation and growth rate of each newly generated fracture is then a function of the local stress field at the selected center. Networks generated by this so-called "stress-driven UFM model" are found to have fractal correlations. We also perform a lacunarity analysis of fracture densities to quantify the textural heterogeneity of fracture patterns with observation scale. We show that our model brings closer to natural data in terms of spatial variability in comparison with "Poisson models". This heterogeneity in the fractures spatial organization has important consequences on the connectivity and flow properties of the rock mass.

References:

Acceptance of Terms and Conditions:

Click here to agree
Poster 3 / 296

A systematic study flow on microscopic pore structure and fluid flow mechanism of tight gas reservoir

wenjie zhang1; yongfei yang1

1 china university of petroleum

Corresponding Author(s): zhangwenjie_2016@163.com

As one of the most important energy resources, improving the recovery of tight gas reservoir will be of great significance. However, the complicated pore structure and special fluid flow mechanism makes it difficult to study with usual experiment methods. To address this problem, a systematic experiment procedure is proposed and applied to Sulige tight gas field. First, the pore structure is obtained with the method of low-resolution CT scan which can get pores diameters above 1 and high-resolution focused ion beam scanning electron microscopes (FIB-SEM) which can reconstruct 3D structure using mathematical method. Mercury intrusion porosimetry (MIP) with a detection range from 3 to 1000 . This combination makes sure that the measure can cover the whole range of pore size distribution. Then, pressure sensitivity, water-sensitive damage and water-gas flow experiments are applied to estimate the flow characteristic and supply data to complement numerical study. After this, the pore network model is extracted from the digital core. Tight gas flow mechanism is studied through Lattice-Boltzmann method which can supply the relative permeability and capillary curve. This case study provides a work flow to analysis pore structure and pore-scale flow of tight gas rock and will be helpful to the development of tight gas reservoir.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-C / 282

A thermal-coupled model of hydraulic fracture propagation in deep reservoir

Author(s): Wenzheng Liu1
Co-author(s): Jun Yao1; Qingdong Zeng1

1 Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China)

Corresponding Author(s): upc_lwz@163.com

Abstract: With the increasing demand of oil and gas resource in the world, the development of deep reservoir has become an inevitable trend. In order to investigate the coupled effects of rock elasto-plastic deformation, fluid flow and heat transfer in the process of hydraulic fracturing of deep reservoir, the mathematical model of hydraulic fracture propagation is established based on cohesive zone model (CZM) and embedded discrete fracture model (EDFM). The constitutive equation incorporating thermal stress is derived by using Drucker-Prager yield condition and the associated flow law. Fluid flow in the fracture is modeled with lubrication theory. The thermal non-equilibrium theory is employed to describe the heat exchange between rock matrix and fluid in the fracture based on EDFM. The CZM is used as fracture propagation criterion. Finite element method is used to solve the rock deformation equation. The thermal field and fluid flow in the fracture are modeled with finite volume method. Due to the non-linearity of flow equation, an iterative method is adopted to solve the coupled problem of stress, pressure and thermal fields. A Triangular-PEBI (Perpendicular Bisector) dual mesh system is presented for numerical implementation. The numerical model is validated against with analytical solution and other methods in the literature. The results show the significance of accounting for elasto-plastic deformation and heat transfer when simulating hydraulic fracture propagation in deep reservoir.
Keywords: deep reservoir; hydraulic fracturing; elasto-plasticity; heat transfer; cohesive zone model; embedded discrete fracture model

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 81

A tri-phase phase-field model for precipitation and dissolution in partially saturated porous media

Magnus Redeker¹ ; Christian Rohde¹ ; Iuliu Sorin Pop²

¹ University of Stuttgart
² Hasselt University

Corresponding Author(s): sorin.pop@uhasselt.be

We consider a porous medium where the pore space is completely filled by three different phases: two immiscible fluids like water and air or oil and a solid phase. The non-wetting phase contains no solute and has no interaction with the solid phase. The wetting phase contains dissolved ions, which can precipitate at the pore boundary to form the solid phase. The reverse process of dissolution, is also possible.

The precipitate has a non-negligible size when compared to the pore size. Therefore, precipitation and dissolution can lead to changes in the pore volume available to flow and, at a larger scale, to changes in the porosity of the medium when interpreting the latter as the volume available strictly to fluids. Moreover, these changes are which are not known a priori.

Starting from a pore scale model that involves sharp interfaces between the three phases and incorporates the dynamics at the pore scale, we develop a diffuse interface approach that accounts for the evolution and the spatial distribution of the three phases and the overall concentration of the solute. The model extends the ideas in [2], where only two phases (water and solid) are considered. Some properties of the model are discussed, including its convergence to the sharp interface model when letting the interface width parameter approach 0. Further, assuming that initially the porous medium consists of periodically distributed grains, we employ homogenization techniques to derive a two-scale model that is valid at the Darcy scale. The outcome is a parabolic reaction–diffusion system in a medium with variable, concentration dependent porosity. The evolution of the porosity is given by the phase field equations defined at the pore-scale.

Finally, an efficient numerical scheme for approximating the solution of the two-scale model is presented. This scheme builds on the algorithm in [3]. The numerical results show how the changes in the pore structure, which are due to precipitation and dissolution, and the evolution of the averaged, Darcy scale concentration of the dissolved ions in the wetting phase, influence each other.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-D / 739

A universal surface modification approach to functionalize microchip devices with rocks/soils surface chemistry
Yaqi Zhang¹ ; Amir Sanati-Nezhad² ; S. H. Hejazi³

¹ a. Subsurface Fluidics and Porous Media Laboratory, Chemical and Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada. b. BioMEMS and Bioinspired Microfluidic Laboratory, Department of Mechanical and Manufacturing Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada.

² a. BioMEMS and Bioinspired Microfluidic Laboratory, Department of Mechanical and Manufacturing Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada. b. Centre for Bioengineering Research and Education, University of Calgary, Calgary, AB T2N 1N4, Canada.

³ Subsurface Fluidics and Porous Media Laboratory, Chemical and Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada.

Corresponding Author(s): yaqi.zhang@ucalgary.ca

The surface chemistry discrepancy between microchips and real rocks/soils restricts the full application of microfluidics technology to subsurface energy and environmental research. Here, we creatively rebuild rock/soil surface chemistries in microchips by forming mineral coatings with an advanced coating technique - layer-by-layer (Lbl) assembly technology. The outcome of this work is a series of ‘surface-mimetic micro-reservoirs (SMMR)’, which represent multi-types and multi-scales of rocks/soils with corresponding rock surface chemistry (e.g., chemical compositions, wettability and surface roughness). Microchip devices made of polydimethylsiloxane (PDMS), glass, Poly(methyl methacrylate) (PMMA) and Norland Optical Adhesive (NOA) are employed for the surface modification and the subsequent surface characterizations and two-phase flow experiments. The morphological and structural properties of the formed mineral coatings are characterized by Scanning Electron Microscopy (SEM), optical microscopy and profilometer; the coating stability is tested by flooding experiments; the surface wettability and roughness are also characterized by measuring mineral oil/water contact angles. The results demonstrate the formation of fabricating material–irrelevant, nano to micro scale, fully-covered and stable mineral surfaces in microchips. In addition, two-phase flow experiments are conducted in the developed SMMR to demonstrate one application of studying the fluid dynamics in subsurface porous media. This work opens horizons for the full applications of microfluidics technology on subsurface energy and environmental research.

References:


Click here to agree

Parallel 2-H / 337

APPLICATION OF LATTICE BOLTZMANN METHOD TO MODEL FLOW THROUGH WATER SATURATED SANDSTONE

Juvenal León-Robles¹ ; Juan Contreras-Pérez¹ ; Graciela S. Herrera² ; Eric Morales-Casique³

¹ Centro de Investigación Científica y de Educación Superior de Ensenada, México
² Instituto de Geofísica, Universidad Nacional Autónoma de México, México
³ Universidad Nacional Autónoma de México

Corresponding Author(s): ericmc@geologia.unam.mx

A numeric model of non-reactive flow through naturally stratified sandstone samples is presented. This work is based on laboratory experiments in which it was established that solute migration in saturated stratified porous media was dominated by stratification. The experiment results strongly suggest that the effect of the stratification is dominant for flow parallel to the lamination in these sandstones. For flow perpendicular to stratification, the behavior is the expected for a homogeneous medium. In this work, an artificial porous media is built based on the parameters obtained from the experiment samples (sample size, grain size, and porosity). The Lattice Boltzmann method is used for modeling the flow through the samples. The aim is to use this method to compare the results from the model with the ones obtained from the laboratory experiments on real media. The sandstone modeled, consisted of a repetition of layers of i) medium-grained sand and ii) fine-grained sand. The
physical properties of this structure were used as parameters to build the artificial porous media. The results from the LBM flow simulation show that when the flow is parallel to lamination, conditions arise for preferential flow, i.e., fingered flow. This instability is associated with the arrangement of grains of different sizes found in the layers. On the other hand, the model predicts uniform flow when the flow is perpendicular to stratification. It is caused by the fine-grained layers, which diffuse the fluid momentum when it moves through these layers.

References:


Click here to agree

---

**Parallel 8-F / 456**

**About front dynamics and up-scaling multiphase flows in heterogeneous porous media**

Benoit Noetinger¹ ; Narges Dashbhesh¹ ; Guillaume Enchéry¹

¹ IFPEN

**Corresponding Author(s):** benoit.noetinger@ifpen.fr

Up scaling techniques allowing to use coarser meshes have rigorous fundations as well as the underlying heterogeneous porous medium presents some statistical homogeneity. In that situation, homogenization theory works well and provides closure problems, the solution of which gives rises to up scaled paramters. These assumptions break down in presence of a front corresponding for example to water flooding of an oil reservoir, or to situations leading to miscible viscous fingering. Breaking translational invariance leads to revisit existing up scaling techniques: it is possible to use standard up scaling far from the front, and to adapt the methods in coarse grid blocks close to the front? It is possible to use effective transport and pressure equations defined at coarse scale accounting for subgrid heterogeneities? It is possible to get a deeper understanding of the coupling between instabilities and heterogeneities?

In that presentation, we will present some approaches and some existing results or conjectures on that issue.

**References:**


Click here to agree

---

**Parallel 8-G / 228**

**Accuracy of WENO and Adaptive Order WENO Reconstructions for Solving Conservation Laws**
Author(s): Xikai Zhao
Co-author(s): Todd Arbogast ; Chieh-Sen Huang

1 University of Texas
2 University of Texas at Austin
3 National Sun Yat-sen University

Corresponding Author(s): xzhao@math.utexas.edu

Weighted essentially non-oscillatory (WENO) schemes can be used to solve the equations governing transport in porous media. They are also useful in defining slope limiters for discontinuous Galerkin and other finite volume or finite difference methods. WENO reconstructions are a weighted average of polynomial approximations defined on various grid stencils. They are designed to produce high order accuracy on the big stencil when the solution is smooth and, when there is a shock, reduce to the order of the approximation on the smaller stencils. This was proven to be the case for the standard WENO reconstruction using the standard WENO-JS weighting procedure in 2011. In this talk, we analyze multilevel WENO reconstructions with adaptive order (WENO-AO) using both WENO-JS and WENO-Z weighting. WENO-AO is more flexible to implement in multiple dimensions and on unstructured computational meshes. We also present a new WENO-AO reconstruction. We give conditions under which the reconstructions achieve optimal order accuracy for both smooth solutions and solutions with shocks. The old WENO-AO reconstruction drops to a fixed, base level of approximation when there are shocks in the solution, but the new one maintains the accuracy of the largest stencil over which the solution is smooth. Our analysis in the discontinuous case requires that the smoothness indicators do not approach zero as the grid is refined. We provide a condition to ensure this result, but we also show an example where this can fail to occur. That is, we show that WENO reconstructions can fail to maintain the order of approximation of the smallest stencil over which the solution is smooth. We also present numerical results confirming the convergence theory of the old and new WENO-AO reconstructions, and compare their performance in solving conservation laws.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-C / 82

Accurate Modelling of Counter-current Spontaneous Imbibition in 2D and 3D Geometries

Herwald Elder ; Rafael March ; Florian Doster ; Sebastian Geiger

1 Heriot-Watt University

Corresponding Author(s): hnet1@hw.ac.uk

Counter-current spontaneous imbibition (SI) is an important transfer mechanism that exchanges fluids between the mobile fractures and immobile rock matrix in naturally fractured reservoirs. The current state of the art of modelling SI involves the use of quasi-analytic solutions for symmetric imbibition along a 1D axis. Unlike contemporary simulators which use first order transfer functions based on saturation potentials, the analytical solutions can capture both the early and late time behaviour of SI.

Our research focuses on the accurate modelling of SI in 2D and 3D. No general analytical solutions exist for SI with arbitrary initial and boundary conditions, so an empirical approach was followed. However, analytical solutions exist for SI where the capillary diffusion coefficient (DC) is linear. Hence we investigated how non-linearizing DC impacts the scaling of the recovery during SI. This analysis revealed that, similar to the 1D case, the behaviour in 2D and 3D can be characterized accurately by an early time regime which scales with tn where n varies from 0.4 to 0.5, and a late time
regime which scales exponentially. These temporal regimes were identified from a derivative analysis of the numerically simulated recovery curves during SI. The numerical error was assessed against the analytical solution for linearized SI problems as the simulation of non-linear SI requires highly resolved grids to correctly capture the recovery and determine the scaling of the temporal regimes. The parametrisation of the temporal regimes was achieved by a numerical sensitivity study involving the effect on recovery due to the shape of DC and the aspect ratio (AR) of the matrix blocks.

The parametrisation of the temporal regimes reveal that they are directly proportional to properties of DC such as the maximum of DC, the saturation at which the maximum occurs, the area under the DC curve and the AR of the blocks. The comparison to contemporary first order model shows that our model captures the fluid exchange during SI over the entire time more accurately.

References:
Click here to agree

Parallel 4-F / 170

Adaptive Mesh Refinement with the Enhanced Velocity Mixed Finite Element Method for Multiphase Flow

Benjamin Ganis¹ ; Gergina Pencheva¹ ; Mary Wheeler¹

¹ The University of Texas at Austin

Corresponding Author(s): bganis@ices.utexas.edu

In this work we consider a mixed finite element formulation using the enhanced velocity (EV) method to construct a strongly flux-continuous velocity approximation on spatially non-conforming grids. The EV method was recently generalized to semi-structured grids, in which each subdomain represents its own mesh refinement level of a structured grid with arbitrary inactive cells. The union of all subdomains forms a non-overlapping decomposition of the entire domain, and adaptive mesh refinement allows this decomposition to dynamically change at every time step to locally resolve sharp fronts. This approach will be demonstrated in an equation-of-state compositional flow model.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-G / 835

Adaptive Online Multiscale Model Reduction for Heterogeneous Problems in Perforated Domains

Eric Chung¹ ; Yalchin Efendiev² ; Maria Vasilyeva² ; Yating Wang²

¹ The Chinese University of Hong Kong
² Texas A&M University
Corresponding Author(s): wytgloria@math.tamu.edu

In this work, we develop and analyze an adaptive multiscale approach for Stokes problems in heterogeneous perforated domains. In many applications, these problems have a multiscale nature arising because of the perforations, their geometries, the sizes of the perforations, and configurations. Typical modeling approaches extract average properties in each coarse region, that encapsulate many perforations, and formulate a coarse-grid problem. In some applications, the coarse-grid problem can have a different form from the fine-scale problem, e.g., the coarse-grid system corresponding to a Stokes system in perforated domains leads to Darcy equations on a coarse grid. In this work, we present a general offline/online procedure, which can adequately and adaptively represent the local degrees of freedom and derive appropriate coarse-grid equations. Our approaches start with the offline procedure, which constructs multiscale basis functions in each coarse region and formulates coarse-grid equations. We then develop an adaptive strategy in the online procedure, which allows adaptively incorporating global information and is important for a fast convergence. We present online adaptive enrichment algorithms for the three model problems mentioned above. Our methodology allows adding and guides constructing new online multiscale basis functions adaptively in appropriate regions. We present the convergence analysis of the online adaptive enrichment algorithm for the Stokes system. In particular, we show that the online procedure has a rapid convergence with a rate related to the number of offline basis functions, and one can obtain fast convergence by a sufficient number of offline basis functions, which are computed in the offline stage. To illustrate the performance of our method, we present numerical results with both small and large perforations. We see that only a few (1 or 2) online iterations can significantly improve the offline solution.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 1-A / 774

Adaptive hybrid multilayer model coupling vertically-integrated and full multi-dimensional models for geological CO2 storage

Tianyuan Zheng\textsuperscript{1}; Bo Guo\textsuperscript{2}

\textsuperscript{1} Helmholtz Centre for Environmental Research
\textsuperscript{2} Stanford University

Corresponding Author(s): ichbinzty@gmail.com

CO\textsubscript{2} injection into a saline aquifer leads to a two-phase flow system (supercritical CO\textsubscript{2} and brine), which often involves large spatial and temporal scales that require high computational cost. To address the computational challenge, in the past decade, a series of simplified models based on vertical integration of the full multi-dimensional governing equations have been developed. These vertically integrated models either assume a rapid segregation between CO\textsubscript{2} and brine due to strong buoyancy (i.e., vertical equilibrium assumption) or solve the one-dimensional vertical two-phase flow dynamics as fine-scale problems on top of the (coarse-scale) vertically integrated equations. The former is often referred to as vertical equilibrium (VE) model, while the latter relaxes the VE assumption and is called dynamic reconstruction (DR) model \cite{1,2}. The major computational cost of the VE and DR models comes from solving the coarse-scale vertically integrated equations while the computation associated with the vertical reconstructions (either VE or DR) is minor. As such, they are much more computationally efficient than full multi-dimensional models and have been used to answer many important engineering questions. However, the vertically integrated VE or DR models are often limited to aquifers with homogeneous or layered heterogeneous properties. Thus, for aquifers with strong 3D heterogeneity, the computationally expensive 3D models are to date the only robust option.

In this talk, we present a hybrid multilayer framework to couple full multi-dimensional models with the various vertically integrated models. Such a framework allows us to use full multi-dimensional models in highly heterogeneous layers of an aquifer where full multi-dimensional model is the only
robust option, while applying simplified vertically integrated models in layers with homogeneous or layered heterogeneous properties. We develop algorithms to couple the full multi-dimensional model with vertically integrated models (VE or DR), as well as algorithms for the coupling between the VE and DR models. In addition, we develop a local criterion to adaptively switch between VE and DR reconstructions [3], i.e., use VE reconstructor when the two fluid phases are in equilibrium while use DR reconstructor to capture vertical dynamics when the fluids deviate from vertical equilibrium. Comparisons with full multi-dimensional models (MRST [4] is used in our work) show that our adaptive hybrid multilayer model is much more computationally efficient than full multi-dimensional models while providing results with similar accuracy, making this hybrid model an attractive tool for modeling of CO2 injection and migration in highly heterogeneous saline aquifers.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-G / 805

Adsorption and Transport in Multiscale Porous Media

Benoit Coasne

1 CNRS/University Grenoble Alpes

Corresponding Author(s): benoit.coasne@univ-grenoble-alpes.fr

Hierarchical porous materials such as hierarchical zeolites, which combine several porosity scales, are widely used in industry (adsorption, separation, catalysis) to overcome slow diffusion in microporous solids (< 2 nm) and enhance access to their large surface area. Available modeling approaches for adsorption and transport in such multiscale porous media are limited to empirical parameters which cannot be derived from molecular coefficients. In particular, existing approaches do not offer the ground for a bottom up model of adsorption/transport in multiscale materials as (1) they describe empirically the adsorption/transport interplay and (2) they do not account for the breakdown of hydrodynamics at the nm scale.

In this talk, I will present a multiscale model of adsorption and transport in hierarchical materials obtained by adding mesopores (~ few nm) and macropores (~ 10 nm) to existing microporous crystals. I will first show how adsorption, permeance, and transport in such media can be described without having to rely on macroscopic concepts such as hydrodynamics [2,3]. Using fundamental parameters and coefficients available to simple experiments, we will see how transport coefficients can be rigorously obtained from simple models in the framework of Statistical Mechanics. Then, I will present a multiscale model of adsorption and transport in hierarchical materials [4]. This approach consists of upscaling accurate molecular simulations in a lattice model. Thanks to the use of atom-scale simulations, which capture the different adsorption and transport regimes upon varying the temperature, pore size, pressure, etc. this bottom-up model does not rely on hydrodynamics and, hence, does not require assuming a given adsorption or flow type. I will also discuss NMR experimental results on transport in hierarchical zeolites [5].
Adsorption induced transformations of methane adsorbed in MOF-5

Bogdan Kuchta¹ ; Filip Formalik² ; Lucyna Firlej³ ; Philip Llewellyn¹

¹ Aix-Marseille University
² Wrocław University of Technology Faculty of Chemistry Group of Bioprocess and Biomedical Engineering
³ University of Montpellier

Corresponding Author(s): bogdan.kuchta@univ-amu.fr

At the nanoscale the positions of coexistence lines on the phase diagrams are shifted and their new locations depend mainly on the size and shape of the nano-confinement, the structure of the confining walls, and their interaction with the confined substance. Here we show that it is possible to induce structural transformations in a confined system by simply varying the number of molecules adsorbed in the pore. We found that the mechanism of these novel, adsorption-induced structural transformation in nano-pores differs from the capillary condensation. First, the structure of the confined gas is determined by a competition between adsorption sites attractive forces and intermolecular interaction. Second, at low temperature, the transformation is discontinuous because it is defined by limited number of adsorption sites [1,2]. The confined, equilibrium structures are not characterized by mean positions of molecules but rather by a probability distribution of molecular positions around adsorption centres. This distribution changes when the number of molecules in the pore increases. The character of transformation is temperature dependent: strongly discontinuous at low temperature, it evolves into a continuous transition when the temperature increases. The mechanism of the transformation is also modified when the size of the gas molecules and types of interaction change. In particular, we report the existence of the intermediate phase, observed only above a critical strength of the attractive interactions.

References:

2. Adsorption-Induced Structural Phase Transformation in Nanopores. Kuchta, Bogdan; Dundar, Ege; Formalik, Filip; et al. Angewandte Chemie Published: 2017-Nov-01 (Epub 2017 Nov 01)

Acceptance of Terms and Conditions:
Click here to agree

Adsorption of small molecules in the intermediate structures of breathing MOF
Author(s): Justyna Rogacka¹
Co-author(s): Azahara Luna Triguero²; Filip Formalik³; Sofia Calero²; Bogdan Kuchta⁴

¹ Faculty of Chemistry, Wroclaw University of Technology, Group of Bioprocess and Biomedical Engineering
² Faculty of Experimental Sciences, University Pablo de Olavide, Division of Physical, Chemical and Natural Systems
³ Wroclaw University of Technology Faculty of Chemistry Group of Bioprocess and Biomedical Engineering
⁴ Laboratorié MADIREL

Corresponding Author(s): justyna.rogacka@pwr.edu.pl

MIL-53 is a MOF porous structures which exhibits very pronounced flexibility. As a consequence, adsorption of CO2 causes its reversible structural transformation, induced by the host-guest interactions. Here, we present detailed molecular modeling study of adsorption of CO2 and CH4 in the intermediate structures of the MOF. We use 20 intermediate structures, between the open pore one and the closed pore form of MIL-53, to study adsorption during the “breathing” of the MOF. 18 intermediate structures were prepared using geometrical interpolation (Fig. 1) and they have been optimized using the DFT quantum calculations. Each structure is rigid and it represents an instantaneous non-equilibrium MOF configuration.

RASPA code is used for molecular simulation [2]. Grand Canonical Monte Carlo and Molecular Dynamic methods are applied to calculate isotherms of adsorption and diffusion coefficients at various temperatures. The simulated adsorption in the intermediate structures show differences in adsorption mechanism of CO2 and CH4. The modeling of adsorption in the intermediate structures allows us to analyze the states which are not in equilibrium and are not accessible in conventional adsorption experiments. For better understanding of the interactions model applied during the process of adsorption, we compare our results with experimentally measured isotherms of adsorption.

Acknowledgements:
JR, FF and BK are partially supported by the Polish National Science Center (NCN, grant no. 2015/17/B/ST8/00099. The calculations have been partially performed at the WCSS computer center of The Wroclaw University of Science and Technology, grant no 33.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 677

Advances in reconstruction and analysis of fast dynamic in situ micro-CT data

Author(s): Marijn Boone¹
Co-author(s): Arno Merkle¹; Denis Van Loo¹; Bert Masschaele¹; Thomas De Schryver¹; Veerle Cnudde²; Tom Bultreys³
Over the past decade, laboratory based X-ray computed micro-tomography (micro-CT) has given unique insights in the internal structure of complex porous materials in a broad range of applications, improving the understanding of pore scale processes and providing vital information for pore scale modelling. The non-destructive nature of micro-CT imaging, combined with dedicated X-ray transparent in situ equipment (eg. flow cells, tensile stages, heating and cooling stages) make it possible to monitor a changing pore structure over time in 3D. Recent advances in lab-based micro-CT hardware have pushed the temporal resolution from the hours down to seconds, enabling the visualization of fast dynamic processes and real-time imaging (Bultreys et al., 2016). Dynamic acquisitions however generate a vast amount of raw projection data, which needs to be reconstructed and further post processed. It is therefore key to quickly identify the interesting moments in time prior to reconstruction to optimize the amount of data that is generated, but also incorporated the added time dimension in the 3D analysis workflow to improve image quality.

In this work we present challenges and possibilities in dynamic micro-CT imaging for fast real-time acquisitions, reconstruction and analysis. The methodology and dedicated workflow from acquisition to analysis is illustrated using different flow experiments performed in a custom made X-ray transparent flow cell on limestone, sandstone and sintered glass samples. The first experiment, described in Boone et al. (2016), is single phase solute transport, where during continuous acquisition a tracer salt is injected in the pore space of a limestone sample. The capabilities of dynamic reconstruction of this experimental data is shown and analysis of the resulting 3D images enable distribution mapping of solute in the pore space through time. Other studies to be shown consist of two multiphase flow experiments of drainage and imbibition. In the drainage experiment, described in Bultreys et al. (2015), oil is injected in a brine saturated sandstone and the pore filling process can be visualized. By incorporating the temporal information in the 3D analysis of the pore space, individual pore filling events can be automatically identified and the size of these events monitored. For imbibition, on the other hand, water as wetting phase is injected in a sintered glass sample and the growth of water films and speed of pore filling can be analysed by reconstructing images from different time intervals and merging the appropriate temporal and local information for analysis.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-H / 153

Advances in the modelling of void clusters and transient wettablility

G Peter Matthews¹ ; Giuliano Laudone¹ ; Charlotte Levy¹ ; Katie Jones¹ ; Cathy Ridgway² ; Ingrid Hallin¹ ; S. Andrea Gazze³ ; Lewis Francis³ ; Joachim Schoelkopf³ ; Patrick Gane³

¹ University of Plymouth  
² Omya International AG  
³ Swansea University
Corresponding Author(s): pmatthews@plymouth.ac.uk

We present a major new advance in the interpretation of percolation characteristics, provided by mercury porosimetry, porometry, water retention for soils, and, for nanoscale porosity, Grand Canonical Monte Carlo simulations matched to surface area adsorption measurements. The new method provides a complete analysis of all the void types, providing the user with cumulative distributions that asymptote with size towards the accessible sample porosity. It employs a quasi-Bayesian inverse modelling approach that interprets the percolation characteristic in terms of pores, pore-throats and void clusters, and is shown to be much more accurate than the traditional but incorrect distributions based on the slope of the percolation intrusion characteristic. The advances are applicable to a wide range of micro and mesoporous non-ordered porous materials. Their utility is illustrated by application to three porous materials of current interest: (i) graphite manufactured in Japan for the cores of next generation nuclear reactors, (ii) microporous calcium carbonate being developed for delayed oral drug and flavour delivery, and (iii) naturally occurring hydrophobic soil which will become less fertile and more prone to causing floods under expected climate change conditions. We also describe an improved wetting algorithm, of use not only for soil but also for other important systems such as membranes and fuel cells.

The new void analysis method uses a Boltzmann-annealed amoeboid simplex to inverse model the percolation characteristic. The convergence of the simulated onto the experimental percolation characteristic is automated within the PoreXpert(R) software package [Levy et al. (2015)]. The resulting void structure comprises a ‘unit cell’ with periodic boundary conditions, containing up to 108,000 void features. Since the solution to the inverse problem is non-unique, a series of stochastic solutions is generated, and the most statistically representative structure is chosen. For the graphite, a size-range gap between the derived GCMC and direct mercury intrusion percolation data is reflected in a wider range of stochastic generations due to the uncertainty for voids of around 1μm [Jones et al., 2018]. The percolation characteristic of the representative structure is then forward modelled. A comparison of the intrusion pressure of each pore with respect to the applied pressure then demonstrates whether each feature is a true pore or a cluster of voids [Matthews et al. 2017].

The working equation for the wetting algorithm, derived from that of Bosanquet, is:

\[ x = \left[ \frac{b \left( 1 - e^{-a(t_{\text{full}} - t_{\text{entry}})} \right)^2}{2a \left( t_{\text{full}} - t_{\text{entry}} - (1/a) \left( 1 - e^{-a(t_{\text{full}} - t_{\text{entry}})} \right) \right)} \right]^{1/2} \]

\( a \) and \( b \) are constants defined as

\[ a = \frac{8\eta}{\pi \rho}, \quad b = \frac{P_e}{\rho} + \frac{2\gamma \cos \theta}{\pi \rho} \]

\( x \) is the distance travelled by the liquid front in time \( t \) into a cylinder of radius \( r \), \( \eta \) and \( \rho \) are the dynamic viscosity and density of the wetting liquid, \( \rho \) is the liquid density and \( P_e \) is the external pressure applied at the entrance of the capillary tube. \( \gamma \) is the interfacial tension at the meniscus, and \( \theta \) the contact angle of the intruding fluid with the solid surface. \( t_{\text{entry}} \) is the time when liquid enters a particular pore-throat and \( t_{\text{full}} \) when it becomes completely full. The progress of the many thousands of simultaneous wetting events are found by use of a forward Euler method, which reduces the calculation time from weeks to tens of hours. For the soil, the wetting throughout the network stabilises at a timestep of 10 microseconds, which also then equates to the so-called ‘Haines jumps’ of the wetting front.

With respect to the three materials we answer three specific questions: (i) how does the void structure of the nuclear graphite differ if the manufacturing process is changed to increase the density, (ii) can additional microporosity be generated by packing the microporous calcium carbonate particles, and (iii) how do molecular scale hydrophobicity transitions upscale to cause soil hydrophobicity at core and field scale?

References:
Bosanquet CH, (1923) Philosophical Magazine, 6, 525-531

Acceptance of Terms and Conditions:
Parallel 8-C / 353

Algebraic Dynamic Multilevel (ADM) method for flow in heterogeneous porous media with embedded discrete fractures

Mousa HosseiniMehr¹ ; Matteo Cusini¹ ; Hadi Hajibeygi²

¹ Delft University of Technology
² TU Delft

Corresponding Author(s): m.cusini@tudelft.nl

An Algebraic Dynamic Multilevel (ADM) method [1, 2] for fully implicit simulations of multiphase flow in heterogeneous fractured natural porous media is presented. The fine-scale fully-implicit (FIM) system is obtained following the Embedded Discrete Fracture Modelling (EDFM) [3] approach. A set of nested coarse grids at different resolutions (or levels) is constructed independently for each medium. At each time-step the fine-scale FIM system is mapped to a dynamically selected grid formed by grid-blocks of the previously defined grids. The grid resolution is chosen, independently for each medium, based on a front-tracking criterion that ensures that fine-scale resolution is employed only where most physical interactions take place (i.e., moving saturation front). Mapping between different grid resolutions is performed by employing sequences of restriction and prolongation (interpolation) operators. Finite-volume restriction [4] operators are employed to ensure mass conservation whereas different interpolation strategies are employed for each variable. In particular, multiscale basis functions [5] are considered as pressure interpolators to ensure an accurate interpolation of the pressure field inside coarse blocks.

The efficiency and accuracy of the proposed algorithm is shown through a set of challenging 2D and 3D test cases involving various non-linear physics. The sensitivity of the method to the choice of the coarsening and interpolation strategy is also presented.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 793

An Assessment of Research Gaps Related to Deep Water Wellbore Integrity

Author(s): Mary Tkach

Co-author(s): Mileva Radonjic¹ ; Barbara Kutchko

¹ Louisiana State University
Corresponding Author(s): mary.tlach@contr.netl.doe.gov

In order for a deep-water wellbore to uphold its integrity under high pressure - high temperature conditions, the wellbore must possess complete zonal isolation while surrounded in an extreme environment. Highly variable temperature and pressure ranges, shallow flow zones, as well as potentially corrosive fluids and gasses all present unique challenges to the job of the cement which maintains that zonal isolation. As such, alternative options to mainstream choices often present themselves as attractive avenues of discovery.

As it is of utmost importance to maintain structural integrity under HPHT conditions, cement slurries are pumped downhole to provide zonal isolation and structural support to offshore wells. The wellbore system potentially faces a variety of temperature and pressure fluctuations from the immediate onset. These fluctuations may affect the hydration properties of the cement. It is also important to consider the chemical interactions that the cement may have at the rock-cement interface where potential degradation or annulus gaps may occur further risking a decrease in zonal isolation. This presentation intends to review some of the important issues regarding zonal isolation in HPHT conditions and to highlight critical knowledge gaps in order to generate important research questions.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-E / 547

An Image-based Micro-continuum Pore-scale Model for Gas Transport in Organic-rich Shale

Author(s): Bo Gu¹
Co-author(s): Hamdi Tchelepi ¹

¹ Stanford University

Corresponding Author(s): b guo@stanford.edu

Gas production from unconventional source rocks, such as ultra-tight shales, has increased significantly over the past decade. However, due to the extremely small pores (~1-100 nm) and the strong material heterogeneity, gas transport in shale is still not well understood which poses challenges for predictive field-scale simulations. In recent years, digital rock analysis has been applied to understand shale gas transport at the pore-scale. A widely recognized issue with rock images (e.g., FIB-SEM, nano-/micro-CT images) is the so-called "cutoff length", i.e., pores and heterogeneities below the resolution cannot be resolved, which leads to two length scales (resolved features and unresolved sub-resolution features) that are challenging for flow simulations. Here we develop a micro-continuum model, modified from the classic Darcy-Brinkman-Stokes framework, that can naturally couple the resolved pores and the unresolved nano-porous regions. Gas flow in the resolved macropores is modeled with Stokes equation. For the unresolved regions where the pore sizes are below the image resolution, we treat them as a continuum and develop an apparent permeability model considering non-Darcy effects at the nanoscale including slip flow, Knudsen diffusion, adsorption/desorption, and surface diffusion. This leads to a micro-continuum pore-scale model that can simulate gas transport in 3D shale images. We present case studies to demonstrate the applicability of the model, where we apply the new micro-continuum model to 3D segmented FIB-SEM shale images that include four material constituents: organic matter, clay, granular minerals, and macropore. We populate the model with experimental measurements (e.g., pore size distribution of the sub-resolution pores) and parameters from the literature, and identify the relative importance of different physics on gas production. Overall, the micro-continuum model provides a novel tool for digital rock analysis of organic-rich shale.

References:
Parallel 11-H / 424

An alternative model of multicomponent diffusion based on a combination of the Maxwell-Stefan theory and continuum mechanics

Jan František; Jiří Mkyška

Czech Technical University in Prague

Corresponding Author(s): jiri.mikyska@fjfi.cvut.cz

We present a theory of multicomponent mixtures which does not employ any splitting of component fluxes into convective and diffusive parts. Instead, momentum balance is formulated individually for each component in which both 1) viscous friction within a component, and 2) momentum exchange among different components, are taken into account. While the viscous friction is described using the Newtonian stress tensor, the Maxwell-Stefan theory is used to describe the momentum exchange among different components. When the viscosity is neglected, the model of ideal mixture of ideal gases leads to a hyperbolic system of conservation laws. For the non-ideal mixtures, we obtain a first-order system in a non-conservative form. A simplified version of the model is discretized using a combination of the finite volume method and the mixed-hybrid finite element method. Numerical examples are provided to show typical behavior of the solution of the model equations.

Parallel 2-B / 454

An experimental and numerical pore-scale study of bio-enhanced NAPL dissolution in porous media

Author(s): Fabrice GOLFIER

Co-author(s): Marbe BENIOUG ; Tidjani BAHAR ; Constantin OLTEAN

Université de Lorraine - GeoRessources Laboratory

Corresponding Author(s): fabrice.golfier@univ-lorraine.fr

Nonaqueous phase liquids (NAPLs) are still a major challenge for all traditional groundwater treatment technologies. NAPLs often contaminate the subsurface following an accidental spill or due to a defect in the oil storage tank. These pollutants remain trapped in the form of droplets and / or immiscible clusters within the aquifer, thus constituting a persistent source of pollution that is difficult to decontaminate. Predicting the fate of this pollutant requires characterizing all the mechanisms involved and in particular the biodegradation, which can occur in the vicinity of the pollutant source or further, to the dissolved plume. If a significant research effort has been put into investigating the transport and biodegradation of dissolved contaminants, comparatively very few works (e.g., Bahar et al., 2016) are focused on the study of such processes in multiphase conditions (oil/water/biofilm systems).

In this study, we give an attempt to address this open issue from an experimental and numerical
perspective. First, we illustrate impact of bacteria on dissolution of pure organic phase from micromodel experiments. The experimental set-up is made of a micromodel (i.e. 2D transparent flowcell) used to study the dissolution of oil phase. Changes in toluene saturation are directly monitored from recorded two-dimensional images and dissolved concentrations at the outlet are measured by gas chromatograph. Results of toluene dissolution and biodegradation by a toluene-degrading strain (Pseudomonas putida F1) are compared with experiments in abiotic conditions. In parallel, we present a two-dimensional pore-scale numerical model (Benioug et al., 2017) to investigate the main mechanisms governing biofilm growth and NAPL dissolution in porous media. Fluid flow is simulated with an immersed boundary–lattice Boltzmann model while solute transport is described with an interface reconstruction finite volume approach (Benioug et al., 2015). A cellular automaton algorithm combined with the immersed boundary method was developed to describe the spreading and distribution of biomass. Different conditions are considered (spatial distribution of biofilm, reaction kinetics, biosurfactant production, NAPL toxicity) and their impacts on the dissolution process are analyzed.

References:


Click here to agree

Parallel 8-C / 421

An extension of the fault two-layer reduced model accounting for the flow properties of the core and damage zones

Guillaume Enchéry¹ ; Isabelle Faille¹

¹ IFP Energies nouvelles

Corresponding Author(s): guillaume.enchery@ifpen.fr

Modelling flows within faults is crucial for various applications such as the control of faults on overpressure development or hydrocarbon migration in sedimentary basins, the recovery of hydrocarbon components, subsurface gas storage, and the appraisal of the risk of groundwater contamination following an underground nuclear waste disposal.

Faults can be characterized as extended fractures along which there has been significant displacement of the sides relative to one another. They are rarely only geometrical discontinuities but rather zones of deformed rocks with particular fluid flow properties. Following [Fredman et al, 2007] conceptual model, a fault is mainly made of two parts: the core area and the outer surrounding damage zone. These different parts have specific flow properties that can change over time. For instance, the core part filled by clay can behave as a barrier while the fractured damage zones act as conduits to fluid flow.

Since the characteristic width of faults is much smaller than the dimensions of the surrounding studied area, modelling these objects for flow simulations is not simple and different approaches have been considered.

Reservoir simulators usually define transmissivity multipliers that account for the change of permeability induced by faults, but, intra-fault vertical fluid flows are neglected. To simulate these flows, reduced models have been proposed as a trade-off to avoid
building grids representing the complete 3D architecture of the fault zones, which require specific mesh generators and increase significantly the computing times. These reduced models consist in modelling a fault with one or two layer(s) of interfaces of dimension N-1 immersed in an N-dimensional domain. More precisely, the double-layer approach introduces interfaces on both sides of the fault which are conformal with the neighbouring matrix blocks but non-matching in the middle, thus enabling one side of the fault to slip or to have slip with respect to the other side. Another important ingredient for the aforementioned applications is the choice of a space discretization scheme which should provide a consistent approximation of the fluxes. The grids are indeed usually built following the geological layers leading to distorted mesh elements. The use of such numerical schemes is also essential when coupling flows between the matrix block and the fault area through reduced models containing non-matching interfaces. Previous works have already demonstrated that the hybrid finite volume scheme allows one to perform this coupling properly.

In this work, we propose an extension of the double-layer reduced model to take the flow properties of the fault core more precisely into account. This new model introduces the core part between the two layers in a simplified way where the flow between the two interfaces is assumed to occur only in the normal direction. The hybrid finite volume scheme is again used to discretize the whole system of equations. Numerical examples on faulted sedimentary basins show the ability of this new model to simulate new flow patterns within faults including the one where two fluids flow independently from each other along slip-page surfaces.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-H / 535

An integrated tool for digital rock physics: benchmark results for flow simulations

Sven Linden¹ ; Jens-Oliver Schwarz¹ ; Liping Cheng¹ ; Aaron Widera¹ ; Andreas Wiegmann¹

¹ Math2Market GmbH

Corresponding Author(s): liping.cheng@math2market.de

Because of the current low oil price, the Oil and Gas industry needs to optimize their workflows. Digital rock physics (DRP) is the to determine physical rock properties by performing numerical simulations on 3D scans of rock samples. This innovative technique saves time and money in comparison to conventional lab experiments. Besides the increase in efficiency, DRP also allows insights into the actual processes occurring in the rock samples. It is, therefore, considered a game changer for the oil and gas industry. Imaging and calculation are the basis of DRP. They aim to determine the 3D geometry of pore spaces and mineral phases, and to subsequently simulate various physical processes in these digital objects. To obtain macroscopic rock properties such as permeability, electrical conductivity, diffusivity, and elastic moduli, different steps are involved: the image acquisition with well resolved pore throats (CT-scan, FIB-SEM images, etc.); image processing for noise reduction, smoothing, and segmentation; setting up the numerical experiment; and numerically solving the Stokes equations. For each of these DRP steps, there is more than one method and implementation. For quality control of the DRP solutions, benchmark tests are needed to validate the property estimations. The benchmark
results in comparing different solvers with analytical models and empirical models for flow computations on the microstructures ranging from idealized pipes to digital rocks. The innovative and easy-to-use DRP simulator GeoDict® [2] allows to conveniently quantify the impact of numerical solvers, boundary conditions, simulation platforms, etc. on macroscopic rock properties. GeoDict reports the permeability, as well as the runtime and memory consumption. Local or remote servers, as well as cloud services (e.g. MS Azure) can be tested for performances and quality benchmarks. Automatic result reports and PowerPoint presentation generation are possible. We were able to improve the speed of our flow solvers. This is demonstrated by reproducing the predicted permeabilities from the benchmarks in requiring much shorter run-times.

References:

Click here to agree

Parallel 1-C / 275

An overview of mathematical, physical and computational challenges in chemical enhanced oil recovery

Prabir Daripa¹

¹ Texas A&M University

Corresponding Author(s): daripa@math.tamu.edu

Chemical enhanced oil recovery, specially surfactant-polymer flooding, involves porous media flows of simple and complex fluids through highly heterogeneous formations. We will discuss various models based on systems of partial differential equations which pose a variety of mathematical and computational challenges. We will start a dialogue on these challenges with some possible pathways to address these challenges thereby opening doors for new and challenging problems in this area. Our current efforts to develop high performance numerical methods and results based on these models will be discussed. Effects of various chemical agents on oil recovery as well as various fluid mechanical phenomena including fingering and channeling will presented and discussed.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-E / 488

An ultrasonic study on density and elastic properties of nanoconfined argon

Klaus Schappert¹ ; Rolf Pelster¹

¹ Saarland University, Department of Physics

Corresponding Author(s): rolf.pelster@mx.uni-saarland.de

We have performed ultrasonic measurements on porous glass filled with liquid capillary condensate. Reducing the vapor pressures induces the formation of concave menisci at the pore ends and enables us to vary the adsorption-induced pore pressure in a controlled way [1,2]. Measuring simultaneously
the propagation of longitudinal and transversal waves we evaluate the temperature and the pressure dependency of various quantities. Here we report on changes of the fluid density and of the samples longitudinal modulus. We test different effective medium formulas to obtain information on the intrinsic elastic modulus of the liquid and on its normal pressure at saturation.


References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-A / 883

Analysis of CO2 residual trapping over the range of scales, from field to core to pore scales - Heletz, Israel, pilot injection site

Auli Niemi1; Jacob Bensabat2; Saba Joodaki3; Rasmusson Kristina4; Farzad Basirat5; Maryeh Hedayati6; Zhibing Yang7; Lilyanne Perez8; Stanislav Levchenko9; Alon Shklarnik2; Alexandru Tatomir10; Martin Sauter11; Fritjof Fagerlund12; Ferdinand F. Hingerl10; Sally Benson11; Chin-Fu Tsang12

1 Upssala University
2 EWRE
3 Upssala University
4 Upssala University
5 Department of Earth Sciences, Upssala University
6 Upssala University
7 Wuhan University
8 EWRE
9 University of Göttingen
10 Streamsim Technologies
11 Stanford University
12 Upssala University and Lawrence Berkeley National Laboratory

Corresponding Author(s): auli.niemi@geo.uu.se

Residual trapping is one of the key trapping mechanisms for CO2 geological storage, yet difficult to determine in-situ. The present study addressed determination of residual trapping over the entire range of scales from pore to core to field scale, based on data from Heletz, Israel, pilot CO2 injection site. During 2016-2017 two dedicated push-pull experiments have been carried out at the site for the specific purpose of quantifying the residual trapping in-situ, in a well-characterized reservoir layer at 1.6 km depth. The field experiments use a combination of hydraulic, thermal and/or tracer tests before and after creating the residually trapped zone of CO2 and the difference in the responses of these tests is used to estimate the residual trapping of CO2 in-situ. The first experiment is based on hydraulic withdrawal tests before and after the creation of the residually trapped zone. In this experiment, the residually trapped zone was also created by fluid withdrawal, by first injecting CO2, then withdrawing fluids until CO2 was at residual saturation. In the second test, the main characterization method is injection/withdrawal of water and partitioning tracers, whose recovery with and without residually trapped CO2 in the formation is compared. In the second experiment the residually trapped zone is created by first injecting CO2 and then injecting water saturated with CO2 in order to push away the mobile CO2. The experimental field results have been modelled both with simplified analytical models for guidance and with 'full-physics' TOUGH2 [2] simulators, to match the observations and to obtain values for in-situ residual trapping. The resulting estimates are discussed as well as compared to results from laboratory measurements on rock cores, including their modeling with pore network models. The pore network modeling has been based on laboratory data on rock samples from the site. In the first set of pore network modeling, data such as throat size distribution, permeability and characteristic two-phase flow functions [3] were used to calibrate
the model, while the second analysis was based on actual scanned pore space data [4] along with measured hydraulic values.

References:


Parallel 3-A / 548

Analysis of enhanced gas transport in fractured rock due to barometric pressure variations

Dylan Harp1; John Ortiz2; Philip Stauffer2; Hari Viswanathan2; Dale Anderson2; Chris Bradley2

1 Los Alamos National Laboratory, Earth and Environmental Sciences Division
2 Los Alamos National Laboratory

Corresponding Author(s): jportiz@lanl.gov

Barometric pressure variations are often one of the main drivers of gas transport in fractured rock, a process that is referred to as barometric pumping. Barometric pressure variations are complex, multifrequency signals influenced by latitude, weather, elevation, lunar phase, time of year, and diurnal and semi-diurnal earth tides. However, our results indicate that it is often a subset of the pressure frequencies that lead to the vast majority of transport while the majority of frequencies result in minor or even insignificant transport. Identifying the dominant pressure frequencies for transport allow us to more simply and effectively characterize the potential for gas transport to the surface at different geographic locations. We will present barometric pressure decomposition analyses on gas transport in fractured rock.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-A / 595

Analytical Investigation of the Stability and Universal Scaling of the Transition from Spontaneous to Forced Imbibition in Porous Media

Lichi Deng1; Michael King1
Corresponding Author(s): denglichi.ld@gmail.com

Spontaneous imbibition is an important recovery mechanism in naturally fractured reservoirs as capillary forces control the movement of fluid between matrix and fracture. Imbibition is also important in unconventional reservoirs as the capillary pressure will increase when permeability decreases, impacting fracture fluid imbibition during the fracturing process but also during the soaking period before the initiation of production. However, the classic self-similar solution to spontaneous imbibition is limited in representing physical boundary conditions, as during most physical multi-phase flow conditions flow occurs with contributions from both capillary and viscous forces. In this research, we present a theoretical semi-analytic approach to analyze the transient imbibition process where both capillary and viscous forces exist, and compare it with the self-similar solution. Unlike previous analyses that assume purely counter-current or co-current flow, this research proves that for a more general situation, strict self-similarity no longer exists, although a new universal relationship of imbibition rate versus time is obtained.

The transient imbibition boundary conditions we examine are easily achievable in the laboratory and are also comparable to those that will exist in a reservoir. We consider a model where the wetting phase is maintained in contact with the inlet, and hydrocarbon production is allowed on both ends. The hydrocarbon phase is produced from the outlet at a constant imposed rate. Initially, counter-current spontaneous imbibition caused by capillarity at the inlet dominates. As the flood front propagates, co-current flow gradually increases in importance as does the viscous force. The imbibition rate at the inlet will drop to be equal to a prescribed injection flow rate, after which the forced imbibition state is reached and viscous pressure drop totally controls the flow. Traditional Buckley-Leverett theory can then be applied to analyze the subsequent forced imbibition process. The analytic solution for the transient imbibition process utilizes a fractional flow concept. In the current study, the fractional flow changes with time, as does the ratio of co-current and counter-current fluxes. It will be shown that not all choices of boundary conditions are stable, but that the wetting phase imbibition rate must increase at early time beyond any imposed injection rate to reach a limit of stability. The result of the analysis includes a dimensionless parameter that describes the relative magnitude of capillary and viscous forces at the continuum scale. A universal scaling envelope exists for the limit of stability which may be expressed in terms of this parameter and the dimensionless ratio of imposed fluxes at both ends of the system. Above the envelope, the flow is unstable as capillary pressure will cause the imbibition rate to increase and the dimensionless ratio to decrease. Any point below the envelope is stable and is subject to forced imbibition. The boundary of the envelope is the limit of stability, which describes the overall mechanism of transient imbibition and the relative magnitude of capillary and viscous forces at the continuum scale. This stability limit is different from the result obtained by the assumption of a self-similar solution.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-E / 627

Anomalous thermal expansion of water in clays

Laurent Brochard\textsuperscript{1}; Tulio Honorio\textsuperscript{1}

\textsuperscript{1} Université Paris-Est Créteil, Laboratoire MSME

Corresponding Author(s): laurent.brochard@enpc.fr

Under undrained heating, the interstitial water pressure in clays increases two to three times more than what would be expected according to the thermal expansion of bulk water. The thermal pressurization is typically circa 0.5 MPa/K, that is, thermal pressurization can well exceed material resistance upon heating of a few tens of Kelvin, which is critical for many geomechanical applications. The anomalous thermal expansion of confined water is also observed for other materials, notably silica and cement. In this study, we investigate this phenomenon by molecular simulation and confront the case of water in a model of montmorillonite to that of a Lennard-Jones fluid in a slit pore. The results show that the thermo-mechanical properties (thermal rigidity and thermal expansion) of the
two confined fluids follow similar evolutions both in function of temperature and in function of bulk fluid pressure. In contrast, the bulk fluids have quite different evolutions since water is well known to exhibit negative thermal expansion below 4°C. Accordingly, these results tend to show that the anomalous thermal expansion of confined water is rather due to the anomalous behavior of bulk water. The physical origin of the low temperature behavior of water is generally attributed to the hydrogen bond network. Since this network is highly perturbed in the confined space, this could explain why confined water does exhibit a 'normal' behavior.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 865

Application of Dynamic Pore-Network Modeling in the Study of Air-Water Flow through Thin Porous Layers

Chao-Zhong Qin

1 TU/e

Corresponding Author(s): c.qin@tue.nl

Thin porous layers are seen in many applications such as hydrogen fuel cells and hygiene products, in which air-water flow is of great interest. Navier-Stokes-based direct simulations are very computationally expensive, and even prohibitive for low capillary number flow such as water flooding in hydrogen fuel cells. Alternatively, the pore-network modeling needs much less computational resources, while retaining essentials of pore structure information. In this work, a dynamic pore-network model of air-water flow with phase change has been developed. We focused on water drainage processes through thin porous layers. Three test cases were conducted, namely, air-water flow through a thin porous layer, air-water flow through a bilayer of fine and coarse thin porous layers, and water flooding in the gas diffusion layer of a polymer electrolyte fuel cell with phase change between water and water vapor. We aim to demonstrate the application of dynamic pore-network modeling in thin porous media studies. With the help of the case studies, we particularly discussed the challenge of modeling thin porous media at the average scale, and highlighted the role of phase change in removing liquid water in the cathode gas diffusion layer.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 907

Application of MRI T1 mapping on root soil interactions

Andreas Pohlmeier1; Sabina Haber-Pohlmeier2

1 Research Center Jülich
2 IMC, RWTH Aachen University

Corresponding Author(s): a.pohlmeier@fz-juelich.de

Relaxometric imaging has already been known in MRI of natural porous media and plants for some decades. Mostly T2 maps are determined due to the relatively short measurement time. However, T2 is often accelerated by diffusion processes in internal gradients caused by the high magnetic
field strengths typically encountered in MRI. Therefore, the information can not be unambiguously assigned to pore structure changes. In this work we will show that T1 mapping is more suitable and allows the characterization of water mobility in porous media and the monitoring of flow patterns using paramagnetic tracers. We can show that errors due to cross talk artefacts in multi-slice sequences with short repetition times and inhomogeneous spin density and T2 decay can be overcome by determining a complete T1 map. In doing so we monitor a series of inversion recovery filtered images with different inversion times which are normalized on a reference image with identical settings but no inversion recovery filter.

The validity of the approach is proven by recovering the total amount of a paramagnetic tracer injected in a natural porous medium. In the next step we apply the method to two systems that are of great interest in soil-plant research: First, patterns of water flow and root uptake pathways are visualized by monitoring the motion of a paramagnetic tracer. Using this T1 mapping approach a wide range of tracer concentration manifesting in a broad relaxation time range is accessible. By analyzing the observed accumulation patterns, it is possible to conclude on roots with high or less uptake activity within the same root system.

The second example concerns the detection of zones in the immediate vicinity of the root surface with reduced T1 relaxation times compared to bulk soil. In this zone, called the rhizosphere, the pore system can be altered by plant exudates such as mucilage or root hair growth, which reduce the effective pore size and explain the shorter relaxation time. In summary, the mapping of T1 is a very valuable tool for the study of important root-soil processes such as tracer movement and characterization of water mobility in the rhizosphere.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-F / 594

Application of Sharp- and Diffuse-Front Models for Predicting Mass Gain and Saturation in Fibrous Wicks

Mohammad Amin Faghihi Zarandi1 ; Krishna Pillai2

1 University of Wisconsin Milwaukee
2 University of Wisconsin-Milwaukee

Corresponding Author(s): faghihi2@uwm.edu

Wicking as imbibitional flow of a liquid driven by capillary pressure has been an important topic in different areas from simple applications like air refreshers and lightening torches to high-tech one such as Propellant Management Devices (PMD)[1, 2]. In this research, wicking of a liquid into porous wicks made parallel fibers is investigated. In the first step, we developed a model for predicting the height of liquid front during the wicking process as a function of time using Darcy’s law based on the assumption of single-phase flow below a clear sharp front. Then the theoretically developed model was evaluated by performing mass-gain experiments where it revealed satisfying agreement for the majority of tested wicks. However, the model failed to account for partial saturations in the wicks. Therefore, we tried Richard’s equation to predict liquid saturation. The adapted Richard’s equation for our specific porous wicks is solved numerically in 2-D using COMSOL and analytically in 1-D using Mathematica where we treated the porous wicks as transversely-isotropic porous media. We determined capillary pressure and relative permeability directly from pore-scale simulations in wick microstructure using GeoDict. Also, in order to evaluate the numerical and analytical results for Richard’s equation, we used a new liquid-N2 based freezing technique to determine the saturation level along the wick length experimentally. After including the gravity effect, good agreements between the numerical/analytical predictions and experimental results were achieved in saturation distributions.

References:


Acceptance of Terms and Conditions:
Click here to agree

**Poster 4 / 181**

**Application of multiple-point statistics to reconstructing digital rock**

**Author(s):** Yuqi Wu

**Co-author(s):** Chengyan Lin ; Lihua Ren ; Muhammad Jawad Munawar ; Yang Wang ; Yimin Zhang

**Corresponding Author(s):** wu_yuqi150348@163.com

Building a three-dimensional (3D) porous medium is the basis of carrying out the numerical simulation of the fluid flow. To date, many techniques of constructing porous media have been proposed by scholars. Among them, the multiple-point statistics (MPS) method has a unique merit of reconstructing 3D digital rock because it can reproduce long-range connectivity of pore space. The Single Normal Equation Simulation (SNESSIM) is one of the most commonly used algorithms of MPS. In the SNESIM algorithm, the selection of training image is critical because it contains the basic heterogeneous pore structure patterns. In this paper, a 3D training image is used in order to supply the more real heterogeneity of pore structures. On the other hand, the multi-grid search template is applied for the purpose of capturing the pore structures of different scales and speeding up the reconstruction process. Taking Berea sandstone as a test example, the 3D porous media were reconstructed. The two-point correlation function, pore network structure parameters, absolute permeability, flow velocity and the pressure fields are applied as the evaluation indexes to validate the accuracy of the reconstructed models. The comparison result shows that reconstructed models are good agreement with the real model obtained by X-ray computed tomography scanning in the pore throat geometry and topology and transport properties.

**References:**

Acceptance of Terms and Conditions:
Click here to agree

**Parallel 10-C / 515**

**Applications of standard and mixed Virtual Elements to the simulation of physical phenomena in poro-fractured media**

Andrea Borio¹ ; Stefano Berrone² ; Stefano Scialò³ ; Matias Fernando Benedetto³ ; Sandra Pieraccini¹

¹ Politecnico di Torino
² Politecnico di Torino, Italy
³ University of Buenos Aires

**Corresponding Author(s):** andrea.borio@polito.it

When dealing with poro-fractured media, performing efficient simulations of physical phenomena such as the transport of contaminants, subsidence or computing the hydraulic head distribution can be very challenging due to the high number of possible geometrical configurations that have to be taken into ac-
count. Recently, the flexibility of the Virtual Element Method in dealing with complex geometries has been exploited in order to successfully tackle the mesh generation issues that arise when performing simulations on Discrete Fracture Networks [1–4], that represent the fractures inside rocks as sets of planar polygons intersecting each other in space. These networks are usually randomly generated starting from statistic distributions of the physical properties of the soil and fractures can thus intersect with all sort of configurations, including, for example, the case of intersections that are parallel but very close to each other, or intersect with very small angles. The proposed strategies start from triangulations that are generated independently of intersections and are cut into polygons by the intersections. This allows to apply standard domain decomposition techniques (suitable for a parallel implementation of the code) and to discretize each fracture independently, possibly using different approaches: standard and mixed Virtual Elements have been used, obtaining solutions that can be either strongly or weakly continuous, and very good approximations of the fluxes that enter or leave each fracture at intersections.

References:


Click here to agree

Parallel 9-H / 792

Apriori Error Estimates for the Undrained Split Iterative Coupling Scheme for Coupling Flow with Geomechanics

Author(s): Tameem Almani

Co-author(s): Abdulrahman Mana

Corresponding Author(s): tameem.almani@aramco.com

Recently, the accurate and efficient modeling of flow-structure interactions has gained more importance and attention for both petroleum and environmental engineering applications. Three main coupling approaches exist in practice: the fully implicit, the explicit or loose coupling, and the iterative coupling methods. The first approach solves the two problems simultaneously, and is considered the most accurate one. However, it poses several computational challenges to the underlying linear solver. The second approach, on the other hand, decouples the two problems and is only conditionally stable. In this work, we consider the last approach which combines the advantages of stability and decoupling and lies in between these two extreme by imposing an elegant iterative coupling iteration between the two decoupled problems. Specifically, we will focus on the undrained split iterative coupling scheme which starts by solving the mechanics problem, followed by the flow problem, and assumes a constant fluid mass during the deformation of the structure. The convergence of this scheme has already been established in [1, 2] for the single rate scheme, and in [2] for the multirate scheme (in which the flow problem takes multiple fine time steps within one coarse mechanics problem). Here, we will derive a priori error estimates for quantifying the error between the solution obtained at any iterate and the true solution for the single rate undrained split iterative coupling scheme. The approach we will follow is based on studying the equations satisfied by the
differences of coupling iterates to establish a Banach contraction argument, which is then used to derive the targeted apriori error estimates, and is an extension of the work presented in [3]. To the best of our knowledge, this is the first rigorous derivation of a priori error estimates for the single rate undrained split iterative coupling scheme for solving the coupled Biot system.

References:


Poster 2 / 1104

Automated high accuracy, rapid beam hardening correction in X-Ray Computed Tomography of multi-mineral, heterogeneous core samples

Author(s): Carla Romano

Co-author(s): James Minto ; Zoe K. Shipton ; Rebecca J. Lunn

1 University of Strathclyde

Corresponding Author(s): carla.romano@strath.ac.uk

X-ray Computed Tomography scanning is an innovative procedure that allows the internal structure of samples to be computed in 3D. It has completely revolutionized the way several measurements can be achieved in geoscience, including characterization of petrophysical properties of porous media. In order to provide accurate results, it is, of course, necessary to have high quality scan images, free of artefacts. One of the most problematic artefacts is beam hardening, which, in cylindrical shapes, increases the attenuation values with increasing distance from the centre. Until now, no automatic solution has been proposed for cylindrically-shaped cores that is both computationally feasible and applicable to all geological media. A new technique is here introduced for correcting the beam hardening, using a linearization procedure of the beam hardening curve applied after the reconstruction process. We have developed an automated open source plug-in, running on ImageJ software, which does not require any a priori knowledge of the material, distance from the source or the scan conditions (current, energy), nor any segmentation of phases or calibration scan on phantom data. It is suitable for expert and non-expert use, alike. We have tested the technique on µCT scan images of a plastic rod, a sample of loose sand, several heterogeneous sandstone core samples (with near-cylindrical shapes), and finally, on an internal scan of a Berea sandstone core. This last sample was also scanned using a medical X-CT scanner with a fan-beam geometry, as opposed to a cone beam geometry, showing that our algorithm is equally effective in both cases. Our correction technique successfully removes the beam hardening artefact in all cases, as well as removing the cupping effect common to internal scans. For a Berea Sandstone, which varies in porosity from 19%-20%, porosity calculated using the corrected scan is 20.54%, which compares to a value of 14.24% using the software provided by the manufacturer.

References:


Click here to agree

Poster 4 / 931

**Automatic switching from quasi-static to dynamic geomechanical modeling of friction in rate-state faults**
Ehsan Haghighat\textsuperscript{1}, Ruben Juanes\textsuperscript{2}

\textsuperscript{1} MIT

**Corresponding Author(s):** ehsanh@mit.edu

Earthquake mechanics relies on the ability to simulate frictional failure of faults. One of the dominant characteristics of seismic events is unstable frictional failure, that is, the occurrence of fast runaway slip.

In their seminar work, Dieterich\textsuperscript{3} and Ruina\textsuperscript{4} proposed a mathematical description of friction, the rate and state friction law, which is capable of reproducing stick-slip behavior observed experimentally. The resulting frictional behavior has been analyzed in detail using a fully dynamic description for zero-dimensional (block-spring) models [e.g., 3]. One of the key features of the system is stick-slip displacement, whereby the block is stagnant for the majority of time, with sudden bursts of high velocity and acceleration. This behavior suggests combining a quasi-static (non-inertial) description during the stick phase, and a dynamic description during the slip phase.

In order to properly assess the seismic hazard associated with the earthquake, a dynamic simulation is needed to capture the unstable slip response. However, performing full-scale coupled flow-geomechanics dynamic simulations is a formidable task due to the requirement of using very small timesteps (~ 1ms) within multiple earthquake cycles (~ tens of years). In fact, such an approach would be so computationally intensive that is well out of reach and will continue to be in the foreseeable future.

In this work, we address this challenge by extending a simulation approach of coupled flow-geomechanics of faulted reservoirs by automatically switching from a quasi-static description of mechanics while the faults are locked to a dynamic description when slip occurs. We investigate the proper definition of this switching criterion with zero-dimensional models, and test them on two-dimensional poroelastic models with a strike-slip fault, for which a fully dynamic simulation is feasible. Finally, we evaluate the applicability of a quasi-dynamic formulation (which relies on a viscous approximation of the inertial term [5] during the slip phase) for fully coupled models in realistic three-dimensional geologic structures.

**References:**


Acceptance of Terms and Conditions:

Click here to agree

**Parallel 1-F / 956**

**Average velocity profile in a channel partially filled with a porous medium**

Roel Hernández-Rodriguez\textsuperscript{1} ; Philippe Angot\textsuperscript{2} ; Benoit Goyeau\textsuperscript{3} ; J. Alberto Ochoa-Tapia\textsuperscript{4}

\textsuperscript{1} Universidad Autónoma Metropolitana

\textsuperscript{2} Aix-Marseille Université, Institut de Mathématiques de Marseille, CNRS UMR-7373, Centrale Marseille

\textsuperscript{3} Centrale-Supélec
4 Universidad Autonoma

Corresponding Author(s): jaot@xanum.uam.mx

In this work, it is shown that the one-domain approach (Goyeau et al, 2003) can be used to model precisely the average fluid velocity in a channel partially filled with a porous medium. This conclusion is drawn from the comparison of the averages obtained from the solution of the effective transport equations, with position dependent coefficients, and the ones resulting by direct integration of the local velocity values. These were obtained by the solution of the boundary value problem given by Stokes and continuity equations subjected to the no slip condition at the surface of the solid particles and the limiting walls of the channel. It must be mentioned that the comparison at the transition region between the porous media and the fluid is also very good.

Initially, the methodology was derived for porous media formed by parallel plates. In this way, the local velocity, the average velocity, the permeability and the fluid volume fraction could be obtained by analytical expressions (Ochoa-Tapia et al, 2017). However, recently the same kind of results has been obtained using particulate porous media, which for the comparison required the numerical solution of the fully developed Stokes flow problem in the whole system. In principle, the methodology could be extended for porous media of microstructure as complex as required.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-C / 147

BLOCK PRECONDITIONING IN THE NUMERICAL SIMULATION OF FRACTURED MEDIA

Massimiliano Ferronato\textsuperscript{1} ; Andrea Franceschini\textsuperscript{1} ; Nicola Castelletto\textsuperscript{2} ; Joshua A. White\textsuperscript{3}

\textsuperscript{1} University of Padova
\textsuperscript{2} Stanford University
\textsuperscript{3} Lawrence Livermore National Laboratory

Corresponding Author(s): ferronat@dmsa.unipd.it

Accurate simulation of fault and fracture mechanics is a key component in a wide number of subsurface engineering applications. Faults and fractures are typically treated by modelers as discontinuity surfaces embedded in three dimensional (3D) continuous media. From a mathematical standpoint, they are described as internal boundaries whose behavior is governed by the displacement and stress fields acting on the surrounding continuum. Displacements and stresses are in turn influenced by geometrical features of the domain, thus yielding a strongly coupled non-linear problem where the domain boundary definition is itself part of the solution. Here, we focus on efficient preconditioning techniques for the linear systems arising from the discretization and linearization of the governing equations that describe the mechanics of faulted and fractured geological media based on a Lagrange-multiplier formulation.

The application of the fracture model to large-scale problems gives rise to a set of sparse discrete systems of linearized equations with a generalized non-symmetric saddle point structure. The quality and performance of the preconditioner relies on two factors: (i) the preconditioning of the leading (1,1) block and (ii) the Schur complement computation. In this work, we propose and compare various approximations for both elements.
The preconditioner of the leading block has to be selected among the wide set of choices available for elastic problems, i.e., incomplete factorizations, approximate inverses and multigrid approaches, especially on a parallel environment. On the other hand, the computation of the Schur complement can be addressed by using a sparse approximate inverse of the leading block or a physically-based block diagonal algorithm. The Schur complement must be inverted, thus other possibilities come in. The approximate Schur complement can be solved exactly, or its inverse can be directly approximated by a least-square commutator projecting the displacement variables on the space of the Lagrange multipliers. Some test cases are presented to investigate the computational performance and highlight pros and cons of the proposed approaches. Finally, real-world examples are presented and solved in an HPC environment.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 554

Benchmark Analytical Solutions to Advection-Dispersion in Discrete Fractures Coupled with Multirate Diffusion in Matrix Blocks of Varying Shapes and Sizes

Quanlin ZHOU\textsuperscript{1} ; Curtis M. Oldenburg\textsuperscript{1} ; Jonny Rutqvist\textsuperscript{1}

\textsuperscript{1} Lawrence Berkeley National Laboratory

Corresponding Author(s): qzhou@lbl.gov

The current state-of-the-art modeling approaches for contaminant/heat transport in fractured rock include (1) discrete fracture-network (DFN) and discrete fracture-matrix (DFM) models with the fracture network and matrix blocks randomly generated, (2) numerical models based on conventional dual-continuum models, and (3) analytical models with simplified parallel fractures and slab-like matrix blocks. These models differ in the complexity of the fracture network and matrix blocks, modeling accuracy, and computational efficiency, making it difficult to compare their results through benchmark problems.

We developed several benchmark problems of contaminant/heat transport under different flow (e.g., linear, radial, and dipole) fields and provided corresponding analytical solutions to global advection-dispersion coupled with multirate diffusion in the rock matrix. The benchmark problems consist of (1) a fracture network of one, two, and three sets of orthogonal fractures with varying fracture spacing and (2) matrix blocks of various shapes (slabs, squares, rectangles, cubes, and rectangular parallelepipeds) and sizes bounded by the fracture network. The matrix blocks can be isotropic with the same fracture spacing in each direction and anisotropic with varying aspect ratios.

The multirate diffusion caused by different shapes and sizes of matrix blocks was accounted for by using a unified-form diffusive flux equation for 1D isotropic (spheres, cylinders, slabs) and 2D/3D rectangular matrix blocks (squares, cubes, rectangles, and rectangular parallelepipeds) in the entire dimensionless time domain (Zhou et al., 2017a, b). For each matrix block, this flux equation consists of the early-time solution up until a switch-over time after which the late-time solution is applied to create continuity from early to late time. The early-time solutions are based on three-term polynomial functions in terms of square root of dimensionless time, with the coefficients dependent on dimensionless area-to-volume ratio and aspect ratios for rectangular blocks. For the late-time solutions, one exponential term is needed for isotropic blocks, while a few additional exponential terms are needed for highly anisotropic blocks. These solutions form the kernel of multirate and multidimensional hydraulic, solute, and thermal diffusion in fractured reservoirs.

The transient flux equation for multirate diffusion was transformed to develop the analytical solutions to the benchmark problems in the Laplace domain with typical functions (e.g., Airy functions) for the global advection-dispersion equation. The benchmark solutions can bridge the gaps between the three modeling approaches with reasonable complexity of fracture network and matrix blocks, as
well as high modeling accuracy and efficiency. They are very useful for benchmarking the DFN/DFM modeling, whose accuracy depends on how to capture the fracture-matrix diffusive transfer and diffusion within each matrix block.

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 113

Benchmarking of the Density Functional Theory Methods for Accurate Description of Structural Properties in Metal-Organic Frameworks

Filip Formalik1 ; Michael Fischer2 ; Justyna Rogacka3 ; Lucyna Firlej4 ; Bogdan Kuchta5

1 Group of Bioprocess and Biomedical Engineering, Faculty of Chemistry, Wrocław University of Science and Technology, Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology
2 Crystallography Group, Department of Geosciences, University of Bremen
3 Wrocław University of Technology Faculty of Chemistry Group of Bioprocess and Biomedical Engineering
4 Charles Coulomb Laboratory, University of Montpellier
5 Laboratoire MADIREL

Corresponding Author(s): filip.formalik@pwr.edu.pl

Atomic level simulations, such as molecular dynamics (MD), Monte Carlo (MC) or DFT, have recently become indispensable tools for characterization of porous materials [1]. Computational methods are often used to study adsorption, diffusion or separation mechanisms. Here, we perform density functional theory (DFT) calculations of structural properties of flexible and rigid nanoporous MOFs. For the benchmarking for comparison we chose materials from the family of MIL-53 with different metallic centers (Al, Fe, Sc) and flexible materials from the group of zeolitic imidazolate frameworks (ZIF) - ZIF-4, ZIF-8. Additionally, rigid frameworks (IRMOF-1, HKUST-1, Mg-formate and Zn-MOF-74) were added. To describe the interactions in our systems we have selected well-known generalized gradient approximation of exchange-correlation functionals based on PBE functional developed by Perdew et al. [2]. Empirical dispersion corrections (D2 and TS) impact on the selected model was also analyzed [3]. We compared the calculated lattice parameters, bond lengths and angels with well-defined experimental structures obtained from low-temperature X-ray powder diffraction (Fig. 1.). The results of our analysis can help to select the best-describing model for theoretical studies of MOFs and can also be a starting point for other applications of DFT methods such as construction of a force field for MD or MC calculations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-D / 904

**Binding of NaCL during hydration of cement as observed by NMR**

Leo Pel¹ ; Raheleh Pishkari¹

¹ Eindhoven University of Technology

Corresponding Author(s): l.pel@tue.nl

With fresh water becoming scarcer, especially in developing countries, there is a tendency to use sea water for making concrete. Hence, more information on the effect of Na and Cl ions needed on the hydration. During the hydration both types of ions can be chemically bound to cement components, as hydrates are being formed [e.g., Friedel’s salt Ca2Al(OH)6Cl2H2O]. Especially free chloride ions remaining at the end of the hydration can be dangerous, as they have the capacity to diffuse towards the steel bars of the reinforcement, resulting in corrosion.

Using a specially designed Nuclear Magnetic Resonance (NMR) setup, the 1H, 23Na and 35Cl content in cementitious materials can be measured. This setup makes use of a 4.7T magnet. Using a step motor the various inserts can be selected and the 1H, 23Na and 35Cl concentration can be measured quasi-simultaneously. In addition the relaxation of the nuclei can be used to obtain pore-size information, and thereby information on the pore-ion concentration distribution during hydration. In this study we have looked at the hydration of standard cement types, i.e., Portland CEM I and Blast furnace slag cement CEM III with a NaCl solution. The ratio of Na-to-Cl was measured during 48 hours. It is observed that the Na/Cl ratio changes during the hydration, indication a chemical/physical interaction with the cement matrix.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-B / 443

**Biofilms can retain sub-micron fine particles migrating in porous media: toward enhancing durability of bioclogging in soils**

Yong-min Kim¹ ; Tae-hyuk Kwon¹

¹ Korea Advanced Institute of Science and Technology (KAIST)

Corresponding Author(s): amiamam@kaist.ac.kr

With the increasing demands for sustainable and eco-friendly soil improvement methods, utilization of microbial activities in subsurface has received increasing attention as an way to modify and control the mechanical and hydraulic properties of soils. Many bacteria can produce biofilms, which are matrices of organic materials consisting of microbial cells and extracellular polymeric substances (EPS). The formation of biofilms in soil can cause pore clogging, hence reduce the permeability by several orders of magnitude. Therefore, stimulating the biofilm formation has been proposed as a method to seal cracks and leakage in earth structures, such as embankments, dams, and levees. However, because of the possibility of biofilm removal or degradation over time, the durability of biofilms over a long period has been questioned, and this has been hampering the implementation of biofilms in field-scale engineering practices.

Herein, we explored the feasibility of using submicron fine particles to maintain or even enhance
the clogging and permeability reduction in coarse sands. It was hypothesized that biofilms could trap and retain fine particles in their matrices, and this is expected to increase the durability of the induced clogging. To test this hypothesis, we performed the control test and the bentonite slurry injection test. Bacillus subtilis were chosen as model bacteria. In the control test, B. subtilis were cultured and stimulated to form biofilms formation in a clean sand pack while monitoring the permeability. The permeability was reduced by ~50% after 1–2 weeks of experiments, and de-ionized water was injected to test the possible degradation and removal of biofilms. In the slurry injection test, upon the biofilm formation and ~50% permeability reduction following the control test, 1% bentonite slurry was injected. It was found that the injected bentonite particles were effectively attached or retained in biofilm matrices, resulting in slight but additional reductions in permeability. Upon the completion of slurry injection, de-ionized water was again injected to examine the durability of the clogging. This study showed that the biofilms is effective in retaining sub-micron fine solid particles in an aqueous phase, and this provides a valuable basis in biofilm utilization in many civil engineering practices.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 4-D / 886

Bridging Micro and Nano Scales in Fuel Cell Electrodes Using Multi-modal Imaging and Scale-Bridging Modeling

Jiangjin Liu†; Iryna Zenyuk

† Tufts University

Corresponding Author(s): jiangjin.liu@tufts.edu

Polymer-electrolyte fuel cell (PEFC) is a promising energy conversion technology with high thermodynamic efficiency, power density and zero-emission. Due to their low cost and material abundance, PGM-free electrodes are promising candidates for meeting 2020 cost targets set by U.S. Department of Energy (DOE).

However, to compensate the lower volume-specific activity, these catalyst layers are about an order of magnitude thicker compared to conventional Pt-based electrodes. Due to larger thickness, mass-transport and Ohmic losses can be significant within these PGM-free electrodes. Previous modeling efforts, which treat catalyst layer as a porous media with effective properties obtained with imaging methods (FIB-SEM, X-ray tomography), lack in capturing through-thickness morphology inhomogeneity. To better understand the influence of the electrode microstructure on the transport processes, we bridge micro and nano-scales obtained with X-ray computed tomography (CT) to model the transport processes in the PGM-free electrodes.

Two iteration algorithms for modeling scale-bridging between imaged morphology with micro X-ray CT and nano X-ray CT are presented. Micro X-ray CT can capture larger cracks and morphological inhomogeneity. Nano X-ray CT with higher resolution serves as a powerful tool to characterize the meso and nano-scale, which cannot be captured by micro X-ray CT due to imaging resolution limits. In both algorithms, the micro-scale domain is discretized in z-direction into a finite grid, where the effective properties of each grid cell are computed with nano-scale model at each iteration step. Furthermore, the micro- and nano-scale models are linked through boundary conditions. The algorithms work for Poisson’s equations, where two boundary conditions are needed to solve the ODEs. In algorithm 1, micro-scale model generates Dirichlet boundary condition on node i and Neumann boundary condition on node i+1 for nano-scale model to compute the Dirichlet boundary condition for node i+1. Then this Dirichlet boundary condition is fed back to micro-scale model to renew the Neumann boundary condition on node i+1 until solution convergence is reached. In algorithm 2, micro-scale model generates Dirichlet boundary conditions on both sides of the element and passes them to nano-scale model to compute the Neumann boundary condition for node i+1. Then this information is fed back into micro-scale model to update the Dirichlet boundary condition on node i+1. The procedure repeats until the solution converges.
Transport processes in idealized geometries are calculated to assess the algorithms’ effectiveness and to study the convergence rate. Then the two algorithms are applied to study the transport processes in the PGM-free electrodes of the PEFCs. A case study with the reaction rate as a function of local concentration has been studied. The spatial variations of the effective transport coefficient and reaction rate have been shown through the numerical results. The effective diffusivity and tortuosity are proved to be not only determined by the geometry of the material, but also influenced by the reaction rate and boundary conditions in the material. The new algorithms fully consider the influence of microstructure and spatial variations.

References:

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-G / 965

Brine-Oil Interfacial Rheological Response to Adjusted Water Chemistry in Berea Sandstone at High Temperature

Kelly Meyers¹; Teresa Reilly¹; Vladimir Alvarado¹

¹ University of Wyoming

Corresponding Author(s): kseidel@uwyo.edu

The effect of sulfate concentration and salinity on wettability alteration and crude oil-brine viscoelastic interfacial properties at elevated temperature was investigated in this work. Evidence exists that oil recovery can be improved through management of rock-fluid and fluid-fluid interactions. The multicomponent interfacial dynamic response is complex function of brine composition and temperature. Wettability alteration at high temperature was examined in Berea sandstone. Contact angle measurements on a high pressure/high temperature pendant drop system and spontaneous imbibition experiments were conducted on aged (oil-wet) cores at high temperature. Interfacial viscoelastic characteristics of the crude oil-brine interface are concurrently investigated applying a newly developed spinning drop technique. Droplet-size distribution of water-in-oil emulsions were tracked over time through low-field NMR measurements. Four brines were selected to assess the effects of both salinity and sulfate ion, and all measurements were conducted at high temperature to compare with previously collected data at low temperature. Our results provide insights into crude oil-brine and rock-fluid interactions at near reservoir conditions. Carefully designed spontaneous imbibition experiments show that in strongly water-wet media, recovery responses are consistent with changes in the interfacial rheology. Stable oil ganglia maintain connectivity of the oil phase encouraging a low residual oil saturation. While in strongly oil-wet media, wettability alteration could dominate fluid-fluid interactions. Subsequently, the higher crude oil-brine viscoelasticity allows the small detached oil droplets to more frequently coalesce forming oil banks, and therefore, contributing to improved oil recovery. Spinning drop results at high temperature show that low-salinity brines produce a more elastic interface than brines with increased sulfate concentrations. Data suggests that excessive sulfate concentrations may resemble properties characteristic of high salinity brines. Droplet-size distribution analysis supports these observations, showing a change from low temperature behavior that correlates with the interfacial viscoelasticity response. Wettability alteration is shown to exist within the experimental system studied in this work, but fails to address the big picture; an underlying coexistent mechanism must be investigated. Fluid-fluid interactions are poorly represented in the literature and as such, the conditions under which each interaction dominates are unclear. The work presented herein provides an initial framework to identify the situationally dominant mechanism.

References:
Parallel 8-B / 670

Bubbles breaking the walls and granular-frictional fingering

Jon Alm Eriksen¹ ; Renaud Toussaint² ; Bjørnar Sandnes³ ; Knut Jørgen Måley⁴ ; Eirik Grude Flekkøy⁵ ; Beny Marks⁶ ; Olivier Galland⁶

¹ University of Oslo, IGPS Univ Strasbourg
² CNRS, IGPS UMR 7516, University of Strasbourg
³ College of Engineering, Swansea University
⁴ PoreLab, Department of Physics, University of Oslo
⁵ PoreLab, Univ Oslo
⁶ Physics of Geological Processes, Department of Geosciences, University of Oslo

Corresponding Author(s): renaud.toussaint@unistra.fr

Experiments on confined two-phase flow systems, involving air and a dense suspension, have revealed highly non-trivial flow morphologies. As the air displaces the suspension, the grains that make up the suspension tend to accumulate along the interface, and can build up force chains that jam the accumulated region. This dynamics will generate “frictional fingers” of air coated by a region of densely packed grains. The fingers have a characteristic width that balances surface tension and frictional forces of the densely packed grains. When these fingers grow under the influence of gravity, they can align either horizontally or vertically, or grow in a random isotropic fashion. The transition between the different modes of finger growth depends on the density of grains, and the gravitational force component. We present an analytic model to account for the transitions between the modes. We further present a numerical scheme that enables us to simulate the dynamics of the process. The numerical and analytic results are in good agreements with the experimental findings. Finally we show how this process could explain patterns that emerge naturally in early stages of dyke formation. These patterns are formed when hot fluid displaces partly molten rocks and packs the hard mineral grains composing it together, thereby forming finger structures that remain frozen in the dyke walls.

We also show how bubbles of gas stabilized by frictional fingers in negligible gravity lead during the rise of overpressure to hoop stresses in the bubble frictional environment, that eventually buckles and destabilizes, and allows the bubbles to break their confining walls, giving rise to channelling and new bubble expansion.

References:

Parallel 7-C / 952

Buoyant Fluid Flow in Inclined Fractures

zhenyu xu¹ ; Laura Pyrak-Nolte²

¹ Purdue University
² 525 Northwestern Ave, West Lafayette, IN 47907
Corresponding Author(s): xu548@purdue.edu

Natural and injected fluids in the subsurface often vary in composition and have different physical properties such as density and viscosity. It is well known that fracture aperture distributions control flow, transport, and mixing of fluids within a fracture. In this study, the effect of fracture orientation on fluid mixing is examined for two cases with a density contrast (1) between miscible fluids, and (2) between miscible reactive fluids that form precipitates.

Fractures with uniform apertures (~2mm) were formed from transparent acrylic plates (50 mm in thickness).

The transparency of the samples enabled imaging of the flow and transport within the fracture to study fluids and precipitation distribution development during the pumping of two solutions. The two solutions were Na2CO3 and Na2CO3 + NaCl solutions in miscible nonreactive case; and Na2CO3 and CaCl2 solution in reactive miscible case. The reaction for forming CaCO3 precipitate in reactive case is as follows:

\[ \text{CO}_3^{2-} + \text{Ca}^{2+} \rightarrow \text{CaCO}_3(s). \]

Solutions were dyed with pH indicators (Bromocresol green or purple) to help distinguish them. The solutions were introduced through two separate ports using a dual-syringe pump (constant flow rate). Fracture inclination angles were set to be 0°, 15°, 30°, 45°, 60°, 75°, 90° to investigate the different distributions of fluids and precipitation.

The experimental observations found very different distribution of fluids, as well as precipitation, that depended on the inclination of the fracture plane. In the miscible nonreactive experiments, when the fracture is horizontally oriented (inclination angle is 0°), stratification of flow occurred with the lighter solution flowing on top of the heavier solution. Mixing occurred across the entire fracture. When the fracture was vertically oriented (inclination angle is 90°), a mixing interface arose from the bottom of the fracture. The lighter solution formed a continuous narrow flow path from the inlet to the middle of the fracture. Halfway up the fracture plane, a few instabilities occurred resulting in discontinuous bubble-like transport to the outlet. In the miscible reactive experiments, when the fracture is vertically oriented, precipitates only formed along the narrow flow path of the lighter solution. When a fracture was horizontally oriented, precipitate distribution was thick and covered the entire fracture plane. Fracture orientation affects the spatial distribution of precipitate because the mixing interface location is dominated by gravitational effects.

The potential to improve caprock integrity through induced mineral precipitation must account for gravity-driven chemical dynamics that can result in differences in the amount and spatial distribution of precipitates depending on fracture orientation.

This work was supported by the Center for Nanoscale Controls on Geologic CO2 (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

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-F / 779

CAPILLARY DRIVEN MOBILITY CONTROL BY EMULSION INJECTION IN HETEROGENEOUS POROUS MEDIA

Ranena V. Ponce F.1 ; Helena Assaf1 ; Marcio S. Carvalho1

1 PUC-Rio

Corresponding Author(s): poncerv@puc-rio.br

Oil-water emulsion injection has shown significant potential as an Enhanced Oil Recovery (EOR) method. Experimental results revealed that drop size, drop concentration and local capillary number are the most relevant parameters affecting emulsion performance as water phase mobility control agent.

Emulsion injection in real reservoirs and production predictions requires a deep understanding of their flow at the pore scale and the underlying mechanisms responsible for the macroscopic improved oil recovery. Ponce et al. (2017) developed a macroscopic model to describe emulsions flow
in porous media by relative permeability curves parametrization as a function of emulsion concentration and local capillary number.

In this work, we study water alternating emulsion injection (WAE) in a highly heterogeneous reservoir. Parametric analysis was performed in 2D and 3D simulations models to explore WAE performance regarding the time at which the emulsion is injected, the size of emulsion bank and the local capillary number. Results showed that WAE injection may attain an extra oil recovery up to 7% when compared to water injection.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-C / 821

CFD-DEM Modeling of Fracture Initiation Induced by Fluid Injection

Zhuang Sun¹ ; D. Nicolas Espinoza¹ ; Matthew Balhoff²

¹ The University of Texas at Austin
² University of Texas at Austin

Corresponding Author(s): zhuangsun@utexas.edu

The fluid injection involved in CO2 sequestration will result in a change in formation pressure and stress state, which may induce fracture initiation and pose a danger to the long-term secure carbon storage. This work attempts to study fracture initiation based on grain-scale fluid-rock interactions.

CFD-DEM model involves the discrete element modeling (DEM) of solid granular medium and the computational fluid dynamics (CFD) modeling of fluid flow. CFD-DEM model is coupled with bonded-particle model (BPM) to mimic the cement that bonds the framework grains. The numerical model is implemented by coupling the open source discrete element code LIGGGHTS and the CFD toolbox OpenFOAM. The resolved CFD-DEM approach that models the solid phase using the fictitious domain method can capture the particle-particle/fluid interactions even at high particle concentrations. Two benchmark problems with analytical solutions are used to verify the resolved CFD-DEM approach: (1) a falling spherical particle in a fluid and (2) pressure drop through a random packing.

We generate a three-dimension random granular packing that is subjected to constant boundary stresses and vertical drag forces from miscible fluid flow injection. Fracture initiation manifests through either a cluster of bond breakage caused by the drag force exceeding the local skeletal force or opening-mode particle displacement depending on the cementation degree. The fluid flow localization caused by positive feedback at weak points related to local heterogeneity promotes fracture initiation. A regular packing with no weak point under a similar initialization inhibits fracture initiation. Fracture initiates from the artificial defect placed in the center and propagates perpendicularly
to the minimum stress under the anisotropic principal stresses. The fracture evolution in the unconsolidated particle packing is similar to experiments in uncemented sediments. Sensitivity analyses are performed for physical properties and operational parameters including fluid viscosity, grain and cement micromechanical properties, principal stresses and injection velocity. This work, for the first time, uses the resolved CFD-DEM approach to study how particle-scale processes contribute to the injection-related fracture initiation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 833

CO2 Breakthrough Pressure in Resedimented Caprock Seals

D. Nicolas Espinoza¹; J. Carlos Santamarina²

¹ The University of Texas at Austin
² King Abdullah University of Science and Technology;

Corresponding Author(s): espinoza@austin.utexas.edu

Structural trapping is the ultimate barrier for reducing the risk of leaks at CO2 storage sites. Small pores in high specific surface clay-rich caprocks give rise to high capillary entry pressures and high viscous drag that hinder the migration of buoyant carbon dioxide CO2.

In this work we show measurements of the CO2 breakthrough pressure and ensuing CO2 permeability through sediment plugs prepared with sand, silt, kaolinite and smectite. Our experiments and data from the literature demonstrate that the breakthrough pressure can reach ~6.2 MPa in argillaceous formations, and 11.2 MPa in evaporites. The CO2 relative permeability after breakthrough increases up to a maximum of ~0.2. Our parametric study highlights the inverse relationship between breakthrough pressure and pore size, as anticipated by Laplace’s equation. In terms of macro-scale parameters, the breakthrough pressure increases as the sediment specific surface increases and the porosity decreases.

In addition, we introduce two dimensionless numbers that help pre-assess the safety of storativity conditions in-situ. The "sealing number" and the "stability number" combine the initial fluid pressure, the buoyant pressure caused by the CO2 plume, the capillary breakthrough pressure of the caprock, and the stress conditions at the reservoir depth; these two numbers provide a rapid assessment of potential storage sites.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-G / 277

CO2 Foam Displacement Behavior in a Water/Oil Saturated Homogeneous Porous Media

Dongxing Du¹; Yingge Li²; Lichen Zheng¹

¹ Qingdao University of Science and Technology
² Qingdao University of Science and Technology
Corresponding Author(s): du-dongxing@163.com

In relation with the potential applications of CO2 foam technology on Enhanced Oil recovery and carbon geological storage, the paper experimentally and numerically investigated the foam assisted CO2 displacement process in a water/oil pre-saturated porous media. Computational Tomography (CT) technology is employed to visualize the transient sweep process of CO2 foam flow in porous media and the three phase saturation distributions along the sample core are obtained through double-energy CT scan scheme. Studying parameters for laboratory research include type of internal phase of foam fluid, the system pressure and the permeability of the porous media. It is found the foam fluid could push most of the liquid phase content in the latter part of the porous media but leaves the forepart of the sample less flooded, showing a clear entrance effect for foam propagation process in porous media. Compared to the CO2 foam, the inlet behavior for N2 foam is even more profound. The pressure loss for CO2 foam flow is much higher in lower permeable porous media of 179md, which in turn leads to higher oil recovery rate of 10.3% versus 6% in high permeable core samples of 3500md. Due to the increased CO2 solubility, elevated system backpressure leads to less pressure drop for CO2 foam flooding processes without compromising the oil displace capability of CO2 foam fluid. Through introducing the novel stochastic bubble population balance model, which employs only two parameters of bubble generation rate of Kg and the maximum bubble number of n∞, numerical investigations are also carried out concerning foam displacement behavior in porous media. The distribution characteristics of pressure, water saturation and bubble density are analyzed to reveal in mechanism the experimental observed inlet behavior for foam flow in the porous media. Parametrical numerical studies indicate higher Kg values could significantly suppress the entrance effect for foam flow in porous media, whereas the increased n∞ values have little effect on the water saturation distribution in the entrance region of the porous media.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-C / 567

CO2 Storage and Enhanced Oil Recovery in Tight Oil Formations: Insights from Laboratory Investigations and Field-Scale Simulations

Jose Torres1, Lu Jin1; Nicholas Bosshart1; Ian Feole3; Lawrence Pekot2; James Sorensen2; Kyle Peterson1; Steven Hawthorne1

1 University of North Dakota Energy & Environmental Research Center
2 University of North Dakota Energy & Environmental Research Center

Corresponding Author(s): jtorres@undeerc.org

Unconventional plays like the Bakken petroleum system (BPS) are the main reason behind the U.S. oil and gas industry renaissance during the last decade. In that period, more than 10,000 wells have been drilled in the Bakken alone, most of them targeting low or ultralow permeability strata. While the hydrocarbon in-place estimates are in the order of hundreds of billions of barrels, most recovery factor estimations range in the single digits. Thus enhanced oil recovery (EOR) has emerged as an area of interest attracting attention from governmental agencies, operators, and academic institutions.

Recently, the Energy & Environmental Research Center (EERC) conducted a comprehensive set of Bakken-centered EOR research activities, including lab experiments, reservoir characterization studies, modeling and simulation exercises, and a field test. Key findings indicate that tight oil formations such as the Bakken may be suitable targets for CO2 EOR opportunities. The use of CO2 serves a twofold purpose: CO2 is an excellent hydrocarbon extraction solvent, and CO2 sequestration contributes to mitigating greenhouse emissions.
This work presents a systematic modeling and simulation study that incorporates freshly acquired laboratory and field data sets from the Bakken Formation. The goal of these efforts was to better understand the implications of injecting CO2, CO2 storage efficiency, oil mobilization and sweep efficiency, and the potential for incremental oil recovery through various schemes.

Core plug-scale measurements were used to calibrate physicochemical parameters of the organic shale members of the BPS. Simulations replicating hydrocarbon extraction experiments using supercritical CO2 allowed the assessment of mass transfer mechanisms at work. The results indicated molecular diffusion and CO2 adsorption had significant effects on fluid flowing behavior in these tight rocks.

Operational observations were used to inform drill spacing unit models. Field data included petrophysical properties, reservoir pressure, temperature, fluid saturations, fluid composition, and primary production records. 3D heterogeneous models were built to investigate different injection strategies with two contiguous, hydraulically fractured, horizontal wells. Sensitivity studies were performed to quantify the effects of key parameters. Several scenarios were examined in detail, including varied well configurations (vertical or horizontal), well schedules, and targeted injection/production rates. Simulation results obtained with the geocellular models revealed natural fracture networks could result in more favorable CO2 storage and oil sweep efficiency in tight oil reservoirs. The natural fractures may significantly increase the contact area between the formation and the (artificially) stimulated region, leading to more favorable conditions for the recovery process. Consequently, reservoir characterization emerged as a critical element to understand the effectiveness of CO2 storage and enhanced recovery for tight oil formations.

This work improves the understanding of the physical and chemical mechanisms occurring in tight oil reservoirs undergoing CO2 EOR. The simulation models and results provide critical assistance for planning and optimizing both oil production and CO2 storage in future efforts.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-A / 690

CO2 convective dissolution controlled by temporal changes in free-phase CO2 properties

Seyed Mostafa Jafari Raad1; Hamid Emami-Meybodi2; Hassan Hassanzadeh3

1 PhD
2 Pennsylvania State University
3 University of Calgary

Corresponding Author(s): emami@psu.edu

Understanding the factors that control CO2 convective dissolution, which is one of the permanent trapping mechanisms, in the deep saline aquifer and associated dynamics of mixing is crucial in the long-term fate of the injected CO2. The present study investigates the effects of temporal changes in the solubility of CO2 at the free-phase CO2/brine interface on the onset of natural convection and the subsequent convective mixing by conducting linear stability analyses (LSA) and direct numerical simulations (DNS). A time-dependent concentration boundary is considered for the free-phase CO2/brine interface where the CO2 concentration first decreases with the time and then remains constant. The LSA results show that the temporal variation in the concentration increases the onset of natural convection up to two orders of magnitude. In other words, size and pressure of the injected CO2 affect the commencement of convective mixing. Based on LSA results, several scaling relations are proposed to correlate critical time and its corresponding wavenumbers with time-dependent boundary’s parameters, such as concentration decline rate and equilibrium concentration ratio. The DNS results reveal that the convective fingering patterns are significantly influenced by the variation of CO2 concentration at the interface. These findings improve our understanding of CO2 solubility
trapping and are particularly important in estimation of potential storage capacity, risk assessment, and storage sites characterization and screening.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 598

CO2 interaction with shale: Insights from experiments and literature

Author(s): Dustin Crandall
Co-author(s): Ernest Lindner; Johnathan Moore

1 U.S. Department of Energy National Energy Technology Laboratory
2 AECOM and the National Energy Technology Laboratory
3 AECOM

Corresponding Author(s): dustin.crandall@netl.doc.gov

Unconventional shale reservoirs with high organic content and swelling clays may have a high affinity for uptake of carbon dioxide (CO2). The pore space and mineral surfaces that sorb/contain petroleum are also potential sorption sites for CO2 and could become available for CO2 uptake once the reservoir is produced and depressurized. Understanding how shales interact with CO2 is important for enhanced resource recovery in the near term, and potential geologic carbon sequestration in the long term.

A series of experiments are discussed where fractured Bakken and Marcellus shale samples were exposed to CO2 at in-situ conditions for extended periods, a computed tomography scanner was used to visualize changes in structure, and simultaneously the fracture permeability was recorded. These measurements allowed for the correlation of hydro-mechanical changes in the fracture which are inferred to be a result of matrix swell and aperture closure.

A detailed examination studies in the literature to extend these results beyond two small samples is then presented. From the experimental CO2/shale interaction results and the growing body of literature on this topic several salient recommendations are presented to unify shale interaction study results into results that can be expanded beyond individual studies. This includes more rigorous characterization of sample constituents, maintaining micro-fabric of the samples, and enhanced control of initial shale water content.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-A / 828
Calcium carbonate precipitation and strontium co-precipitation in porous media flow reactors

Author(s): Neerja Zambare
Co-author(s): Ellen Launchnor ; Robin Gerlach

1 Montana State University

Corresponding Author(s):

Strontium-90 (Sr-90), a toxic and carcinogenic radionuclide, is the product of uranium fission and is found in soil and groundwater at numerous DOE sites. Sr can also enter the environment through mine tailings leachate, produced water ponds (oil and gas extraction) or can occur naturally in rock formations.

A potential technology for groundwater remediation is the use of subsurface microorganisms to induce calcium carbonate (CaCO3) precipitation resulting in the partitioning of metal contaminants into CaCO3 precipitates for long-term sequestration. Precipitation can be facilitated by an increase in alkalinity as a result of urea hydrolysis, which can be induced by microbes in a process called microbially induced CaCO3 precipitation (MICP). Thus, Sr co-precipitation studies have the potential to provide insight into Sr-90 partitioning into CaCO3.

Our studies in three flow systems have aimed to characterize and control CaCO3 distribution and Sr co-precipitation through MICP by manipulating fluid flow and CaCO3 saturation conditions. First, the effects of flow rate and Ca-concentration on the strontium partition coefficient (DSr) were determined in porous media flow cells (FC), similar to those described in Launchnor et al.1 Second, spatio-temporal analysis of strontium partitioning was performed using a novel modified flow cell; this spatially-sampled flow cell (SFC) enabled fluid sampling from different locations within the porous medium during the experiments. Finally, a laboratory-scale reactor, wherein glass beads formed a packed porous bed, was used to investigate MICP under radial flow conditions.

Two flow rates and two calcium concentrations were studied in the FC. The calcium precipitation rate in FC experiments suggested that under the conditions chosen, MICP was limited by calcium transport. The low calcium concentration and low flow rate experiment led to the highest MICP efficiency and Sr co-precipitation.

SFC experiments revealed that calcium and strontium gradients did not remain constant over time. Spatially collected samples aided in DSr calculations to study the spatio-temporal behavior of strontium co-precipitation. The calcium precipitation rate decreased with time in all three replicates. A decrease in strontium partitioning with distance into the SFC was coupled with an increase in the size of the precipitates.

For effective field employment of MICP, it is important to control MICP specifically under radial flow conditions relevant in near-well environments. Porous media radial flow systems were utilized to evaluate spatial distribution of CaCO3. MICP experiments were performed at three fluid flow rates and three calcium concentrations. MICP efficiency showed an inverse relationship to flow rate and the greatest precipitation efficiency was observed at the lowest calcium concentration. Preferential flow paths developed due to precipitates formed via MICP, affecting fluid flow.

These results allow for predicting MICP distribution and the effect of MICP on porous media flow properties and lend insight to potential MICP strategies for remediating Sr-contaminated groundwater.


References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-G / 970
Capillary force under microgravity estimated from Hagen-Poiseuille Equation.

Author(s): Yuichi Maruo

Co-author(s): Naoto Sato ; Kosuke Noborio

1 Graduate School of Agriculture, Meiji University
2 Meiji University

Corresponding Author(s): noboriok@meiji.ac.jp

International Space Exploration Coordination Group plans a long-term human space mission on the Moon or near Earth’s asteroids to make a pass to Mars. Food supply as well as recycling atmosphere and water is one of the largest concerns on the long-term human space mission. Growing plants during the mission in a spacecraft or a base may ease those concerns. Water movement in a substrate is an important factor for plant growth; however, there are few reports on water movement in porous media under microgravity. Our objective of this study is to reveal whether or not Hagen-Poiseuille Equation is applicable under microgravity. To visualize water movement in a capillary tube, 0.8 mm inner diameter tubes were used to observe water movement driven by the capillary force under the 2.5 s microgravity condition made by a free-fall tower. Water movement was captured with a video camera, and water infiltration rates were analyzed by image analysis software. Water infiltration rates in glass tubes under microgravity were much smaller than 1G theoretical value calculated with Hagen-Poiseuille Equation. Capillary force or capillary pressure, which is a main driving force of water movement in glass tubes, was also much smaller under microgravity than 1G theoretical values. These results suggested that, under microgravity, either surface tension, contact angle, or viscosity of water could be different from the 1G condition.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 601

Capillary hysteresis and pore-scale heterogeneity limiting the migration of buoyant immiscible fluid in a porous medium

Author(s): Abdullah Cihan

Co-author(s): Shibo Wang ; Jens T. Birkholzer ; Tetsu Tokunaga

1 Lawrence Berkeley National Laboratory

Corresponding Author(s): acihan@lbl.gov

In geological carbon storage, understanding main mechanisms affecting migration and redistribution of injected CO2 in aquifers is needed for developing predictive models to assess post injection environmental risks and designing long term monitoring schemes. This work presents experimental and modeling studies to investigate processes contributing to post-injection CO2 plume distribution and stabilization. We conducted flow cell experiments (0.5mx0.05mx0.01m) with two fluid phases in macroscopically homogeneous glass-bead porous medium to study post-injection plume behavior. A recently developed hysteretic macroscopic two-phase flow model considering microscale fluctuations in pore size and geometry was used to interpret the experimental results and to understand main processes leading to plume stabilization. Findings demonstrate that both hysteresis and pore-scale heterogeneity control the plume behavior and limit the plume extent. Redistribution of injected plume is extremely slow and occurs through more or less discontinuous jumps over long times. The occurrence of such a phenomenon in real storage formations can make monitoring and assessment of plume stability considerably more challenging. Experimental results at larger more realistic porous media systems are needed to further understand post-injection plume behavior and test post-injection predictive models.
Parallel 5-B / 42

Capillary imbibition in wood governed by water adsorption in walls

Author(s): Philippe COUSSOT

Co-author(s): Denis COURTIER-MURIAS ; Meng ZHOU ; Sabine CARE ; Stéphane RODTS

1 univ. Paris-East
2 Univ. Paris-East

Corresponding Author(s): philippe.coussot@ifsttar.fr

Water transfers through wood structure play a major role in wood behavior under various conditions such as drying, imbibition, sapflow, for which various problems may occur, such as shrinkage, cavitation, fracture, swelling. The physical understanding of these transfers is in some cases rather poor, as illustrated by the fact that it is still sometimes considered that the permeability of wood varies with the sample length, which would mean that it is not an intrinsic material property.

Here we focus on imbibition properties of wood (here hardwood) along the longitudinal direction. We first show that the dynamics of water penetration in hardwood exhibits a contradiction when it is considered within the standard frame of capillary imbibition: on one side we have a very slow dynamics a priori associated with an extremely poor wetting, on the other side the water is finally able to climb at a high level against gravity as for good wetting. This contradiction is confirmed by 3D Synchrotron images of the internal structure obtained during imbibition, which show that the liquid-air interfaces in the capillary vessels remain planar, which implies negligible Laplace pressure, but significantly advance along the vessels, again unexpectedly.

From further examination of the dynamics of water penetration and wood microstructure evolution from Synchrotron images and MRI measurements allowing to distinguish bound and free water, we show that this contradiction is explained by the adsorption of a slight amount of bound water in the cell walls, and at the origin of wood swelling. This adsorption governs the process: it momentarily damps wetting then allows further advance when the walls are saturated with bound water. Finally we definitely prove this mechanism with the help of experiments with model materials, i.e. hydrogels, from which both the ascent of free water and the adsorption and propagation of bound water may be directly observed.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-H / 433

Capillary network simulations based on the centreline representation

Rodrigo Neumann Barros Ferreira ; Peter Bryant ; Ronaldo Giro ; Michael Engel ; Mathias Steiner

1 IBM Research

Corresponding Author(s): rneumann@br.ibm.com
Tomographic 3D imaging at the pore scale provides an accurate geometrical representation of the microstructure of porous networks in oil reservoir rocks. Flow simulation models deployed on top of such geometrical representation unveil a variety of phenomena and allow estimating oil recovery parameters as part of reservoir assessment, management and operation. Physical models based on sparsely-connected graphs have the advantages of high performance and memory efficiency. In this work, we developed a centreline extraction algorithm and used it to characterize the microstructure of the porous network and to build a capillary network simulation that enables the extraction of relevant flow-related figures-of-merit from a 3D image. We do that in a cloud solution environment that facilitates the consumption of those computational tools and infrastructures by stakeholders in the industry.

Starting from the segmented image, the centreline extraction algorithm involves calculating the Image Foresting Transform [Falcão 2004] of the pore space followed by a centrality-aware optimal path algorithm [Cormen 2009] to find the most central path from a pore inlet to a pore outlet. With the resulting centreline graph, we build a capillary network in which every centreline voxel becomes a cylindrical capillary with diameter given by the Euclidean Distance Transform, therefore, reducing drastically (by a factor of 1000) the computational domain and number of variables involved. The Poiseuille’s law is used to establish the relationship between imposed pressure gradient and flow rate in a capillary network simulation [Man & Jing 1999]. Besides the flow-related simulation results, one can extract morphological figures-of-merit from the centreline geometrical representation, such as connectivity, fractal dimension, diameter distribution, length distribution, tortuosity distribution and the correlation between pairs of such properties.

References:


[CORMEN 2009] CORMEN, THOMAS H. INTRODUCTION TO ALGORITHMS. MIT PRESS, 2009. Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-E / 374

Capillary-condensation-induced stress in complex multi-scale porous materials

Edmond Zhou\textsuperscript{1} ; Katerina Ioannidou\textsuperscript{1} ; Enrico Maseoro\textsuperscript{2} ; Mohammad mirzadeh\textsuperscript{1} ; Roland Pellenq\textsuperscript{1} ; Martin Bazant\textsuperscript{1}

\textsuperscript{1} MIT
\textsuperscript{2} New Castle University

Corresponding Author(s): edmondztt@gmail.com

Capillary condensation in a nano-porous material can induce high local stresses affecting its transport, tribological and rheological properties, promoting cracking and can eventually lead to failure of the material.

However it is a non-trivial problem to determine the capillary stress field in realistic 3D structures covering the entire range of degree of liquid saturation.

We propose a general and quantitative numerical framework to address the chemo-poro-mechanics in realistic complex pore networks arising from liquid stresses at all range of relative humidities, exemplified with a mesoscale model of cement.

We discuss the microscopic irreversibility observed in our simulations and its implications on cement drying shrinkage.
Cement placement in damaged shale rocks: effect of shale properties

Nils Opedal¹ ; Malin Torsæter¹

¹ SINTEF Petroleum Research

Corresponding Author(s): malin.torsater@sintef.no

To establish and maintain well integrity to avoid leakage through wells is vital for production wells relevant for the petroleum industry, and for injection wells used for CO2 sequestration. To ensure that stored CO2 remains underground in a long-term perspective it is of the utmost importance to optimize the integrity of both active and abandoned wells. The properties of well barriers such as drilled rock, annular cement and casing steel, and the interplay between them are important considerations during the planning and execution of the drilling phase. Failure of any of these individual materials, including interfaces between them, can lead to leakage.

The bonding quality of cement to rock and steel is thus of crucial importance for long-term well integrity. Several studies have been made of this in the past, but none have taken into account that the drilled rock can be fractured and damaged during drilling. Especially a caprock fractured in the near-well zone can jeopardize well integrity and cause CO2 leakage. In our work we have experimentally investigated the effect of drilling-induced caprock damage on the quality of well cement placement and bonding. Both intact and fractured shale rocks of varying properties was cemented under realistic temperature and pressure, and the quality of the bond was examined using X-ray computed tomography (CT) scanning.

The motivation for this study was to place cement at a wellbore wall with realistic fractures and damage, rather than an ideal wellbore wall with circular cross section. The rock surfaces applied in all previous cement bonding studies were smooth, laboratory prepared rock surfaces. This is unrealistic with respect to a real downhole borehole surface. The shale rock can be damaged by the drill-bit during drilling, or later as a result of impact and smearing from the rotating drill-string and stabilizers. Another important factor is the interplay between the drilling fluid properties and the shale characteristics, which can influence the degree and character of the wellbore wall damage. Since it is of the outmost importance for well integrity that the cement-caprock bond is tight, the ability of cement to seal sufficiently towards realistic shale interfaces is especially interesting to study.

References:

Acceptance of Terms and Conditions:
Click here to agree
Controlling fluid flow through permeable and fractured media is important in a variety of subsurface contexts including geologic carbon storage (GCS). Low pH and or high salinity conditions create corrosive aqueous environments which would rapidly degrade cement in wellbores or carbonate/clay features in caprocks. Our group has explored the potential to deploy dissolution/precipitation reactions using mineral silicates as a way to plug leakage pathways in GCS contexts. Here, we present a combination of experimental and modeling results using wollastonite and pseudowollastonite, which are high temperature polymorphs of calcium silicate, as seed materials to plug leakage pathways. When calcium silicate is carbonated under reservoir conditions it forms calcium carbonate and amorphous silica. But our high temperature and pressure column experiments indicate that in addition to carbonate a number of secondary mineral phases are also possible. Under certain conditions, we observed the formation of crystalline plate- and flower-like mineral hydrates, which formed on fluid-solid interfaces. The type of hydrate that formed was a function of ionic strength, the partial pressure of CO2, the pH of the system, and the type of mineral surface that was available to initiate nucleation of the mineral phases. In column studies, the formation of these mineral precipitates dropped the permeability by several orders of magnitude. These drops could be understood in terms of the significantly larger molar volumes of the products relative to the reactants. These increases in molar volume were significant when normalized to the availability of cations (calcium in this case). These mineral phases were also strong cements that could either improve the mechanical integrity of the rock or add stress to fractures and pores under confined conditions. A proposed mechanism for the chemistry underlying the carbonation of crystalline calcium silicate will be presented and discussed in the context of a reactive transport model to explore the ways in which particles might be injected and carbonated to produce seals in a GCS context.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-G / 1002

Challenges and Opportunities in Porous Media Modeling of Food Materials

Pawan Singh Takhar

Corresponding Author(s): ptakhar@illinois.edu

Foods provide challenging settings for testing porous media physics-based theories. Foods are heterogeneous materials composed of macromolecules such as carbohydrates, proteins, and lipids with continuously evolving structures and material properties during processing. Treating foods as porous materials to model the fundamental transport mechanisms and their effect on product quality is of significant interest to both multibillion-dollar food industry and the consumers. Industry desires at optimizing the food processes to obtain safe and nutritious food products with desirable taste, flavor and texture. However, it is challenging to optimize the food processes by purely experimental approaches due to the involvement of a large number of parameters, difficulties posed by continuously changing material characteristics and dynamic nature of processes. Porous media modeling helps to fill the gaps in understanding the mechanisms and identifying the desired process parameters. For example, during frying of French fries, the structure of potatoes changes from a rigid raw material with high tortuosity to a structure with variable mechanical properties from the center to the surface and low tortuosity. The process involves unsaturated transport of oil, water, vapors and heat with the capillary and pore pressures playing a critical role to affect oil uptake. Besides, thousands of desirable and detrimental chemical compounds are generated during frying. High frying temperatures make instrumental techniques challenging, which leaves a considerable gap in our understanding of the underlying transport mechanisms. In such cases, performing computer simulations with multiscale porous media models allows filling the gaps in our knowledge of
transport mechanisms, keeping track of chemical compounds transport and predicting thermomechanical changes in food biopolymers. While mathematical representation of these materials with multiphases, multispecies and continuously evolving structures has become possible with mixture theoretic approaches, challenges remain on collecting the material properties and validation data. Often a process may be occurring at a temperature much higher than the boiling point of water or at a subfreezing temperature, where property data acquisition by instrumental techniques is limited. It is also challenging to utilize molecular theories due to the involvement of macromolecules for which there is insufficient information on three-dimensional structures. This presentation will discuss some examples of porous media physics’ applications in food science by presenting challenges and opportunities.

References:

Acceptance of Terms and Conditions:
Click here to agree

Invited 2 (Room C) - Mariela Araujo / 1112

**Challenges in Modelling Thermal-Conduction based Hydrocarbon Recovery Methods**

Mariela Araujo¹

¹ Shell International Exploration and Production

**Corresponding Author(s):**

Thermal oil recovery methods have been proposed and progressed for many years as a convenient way to mainly unlock the potential from heavy oil/bitumen accumulations. These methods cover a wide range of techniques like steam/hot fluids injection, in-situ heaters, in-situ combustion, toe to heel air injection etc. A few of them are successful commercially while others are still under development.

Over the past two decades, Shell has executed research programs focused on the development and maturation of in-situ thermal-conduction based methods to recover high quality hydrocarbons from unconventional reservoirs. In this technology solution, heat is injected into the reservoir through a series of heater wells operated at high temperatures. The initial reservoir temperature increases to elevated values around 300°C where thermal cracking of in-situ hydrocarbons and/or enhanced maturation of organic matter takes place, resulting in complex temperature-dependent compositional flow and transport phenomena. At those conditions, most of the fluids in the reservoir are in the vapor phase allowing their recovery through dedicated producer wells. Significant changes are observed in the near wellbore area as the formation responds to the large temperature increase that can negatively impact the production system if not designed properly. Evaluation of the use of the technology relies on the modeling of such process, which is very challenging and computational expensive since it involves the description of these effects occurring in a complex subsurface environment.

This presentation covers: a) an overview of the phenomenology associated with thermal conduction based in-situ methods, b) a discussion on the requirements for the description of the complex associated Physics and Chemistry, c) types of simulation models and numerical tools needed to improve the representation of the observed phenomena, d) alternatives developed to reduce computational requirements of the simulations, e) strategies for hydrocarbon recovery optimization, and f) key focus areas for technology maturation in a commercial development.

The methods and workflows developed were tested in a variety of resources worldwide where Shell gathered extensive laboratory and field data through pilots, providing critical input for model calibration. Examples include in-situ conversion for Colorado and Jordan oil shale reservoirs, evaluation of potential use in liquid rich shale in China, in-situ upgrading for sandstones and carbonates in Canadian heavy oil and bitumen, and could be of interest to other type of unconventional resources.

References:

Acceptance of Terms and Conditions:
Parallel 11-F / 863

Challenges in modelling two-phase flow in industrial porous media

S.M. Hassanizadeh1 ; Amir Hossein Tavangarrad1 ; Hamed AslannejadNone ; Thomas Sweijen1

1 Utrecht University

Corresponding Author(s):

Various industrial processes involve two-phase flow in porous media. Examples are found in fuel cells, filtration, paper, food, concrete, ceramics, moisture absorbents, and membranes, to name a few. The common practice in modelling flow and transport in such porous media is to employ the concepts, models, and algorithms developed in geosciences. However, many industrial porous media are significantly different from soil and flow and transport processes occur in different regimes. Some major challenges are:

- Most industrial porous media are made of a stack of think porous layers. It is not straightforward to measure their material properties, such as permeability and capillary pressure curve. This is because of the small volumes involved in a layers and their deformability.
- Due to their small thickness, there are often only a few pores present across the thickness. So, the applicability of three-dimensional continuum theories is questionable.
- The space between layers is known to affect the distribution of fluids in the layers. It is not clear how such an interlayers space should be characterized and how its effect should be included in a three-dimensional model
- Constitutive relations (e.g., capillary pressure curve) are commonly obtained under equilibrium conditions whereas many industrial flows are very fast.
- Deformations of soils/rocks are infinitesimal or negligible or slow; not always so in industrial flows

There is a clear need for developing theories, models, and measurement techniques specifically applicable to industrial porous media. In this presentation, we highlight the special features of industrial porous media through the discussion of results studies of two industrial applications: penetration of ink into paper and the absorption of liquids in diapers. We also discuss how formulation of two-phase flow in such systems should be modified.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-G / 953

Challenges to understanding water imbibition under microgravity by numerical simulation.

Author(s): Naoto Sato1

Co-author(s): Yuichi Maruo 1 ; Natsumi Naganuma 1 ; Kento Nogawa 2 ; Kosuke Noborio 2

1 Graduate School of Agriculture, Meiji University
2 Meiji University
The ISECG aims to realize the Mars manned space exploration mission in the 2030s. Since the duration of the Mars mission is assumed to be three years, a big concern is how to supply food for astronauts during the mission. The realization of space agriculture may be a solution for food supply problems in space. Understanding a moisture behavior in porous media under various small gravity conditions is indispensable to supply water to plants in space environments. It is reported that an imbibition rate in porous media in the ISS under microgravity was smaller than that of a horizontal infiltration experiment on the ground with 1G. It is suggested that changes in contact angle and the shape of pore throat may inhibit water transfer in porous media under microgravity. Surface tension, contact angle and pore throat shape strongly influence the two-phase flow in a porous medium. The COMSOL Multiphysics software was used for simulating hindered water movement under microgravity. The phase-field method was adopted to calculate energy in the system. We compared water movement in various shapes of pore throat between 1G and microgravity. We also conducted water imbibition experiments under microgravity with a parabolic flight. The results of this experiment will be discussed.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 114

Changing mechanical properties of nanomaterials by surface modification and the impact of capillarity

Author(s): Jürgen Markmann
Co-author(s): Nadiia Mameka

1 Helmholtz-Zentrum Geesthacht

Corresponding Author(s): juergen.markmann@hgz.de

Surfaces may influence elastic and plastic properties of nanostructured materials. Nanoporous gold (npg), as one of the most suitable probes for such effects, was mechanically deformed in an electrochemical environment allowing in-situ modification, i.e. electric charging as well as electroosorption of ion species, while the mechanical loading took place. The change in stiffness in the regime of elastic deformation could be well described by the introduction of a surface excess elasticity resulting in total changes of this parameter of 60 N/m for electroosorption and 12 N/m for capacitive charging of the npg surface. Impressingly, these changes are higher than the total value for the excess elasticity in the range of 8 N/m for uncharged gold surfaces. The surfaces in npg cause considerable capillary forces, in the order of 1 GPa which also influence the plastic deformation behaviour of nanostructured materials. Careful analysis of the observed changes in flow stress in dependence on the applied electric potential allowed us to differentiate contributions of the surface stress and the surface energy. In contrast to current suggestions relying on atomistic simulations which favour the surface stress as the relevant capillary parameter, we observe a significant contribution of the surface energy.

References:
Click here to agree

Parallel 2-A / 836
Chaotic Fluid Advection in Crystalline Granular Media

Régis Turuban¹; Daniel Lester²; Tanguy Le Borgne¹; Yves Méheust³

¹ University of Rennes
² RMIT University Melbourne
³ Géosciences Rennes

Corresponding Author(s): yves.mehheust@univ-rennes1.fr

We study the Lagrangian dynamics of steady three-dimensional (3D) Stokes flow over granular media consisting of simple cubic (SC) and body-centered cubic (BCC) lattices of closed-packed spheres, and uncover the mechanisms governing chaotic fluid advection. Due to the cusp-shaped sphere contacts, the topology of the skin friction field is fundamentally different from that of continuous (non-granular) media (e.g. open pore networks), with significant implications for fluid advection. Weak symmetry breaking of the flow orientation with respect to the lattice symmetries imparts a transition from regular advection to strong chaotic advection in the BCC lattice, whereas the SC lattice only exhibits weak advective mixing. Using a numerical simulation of the flow at various flow orientations, we quantify the strength of chaotic mixing from the Lyapunov exponent, and examine how it is distributed over the parameter space of mean flow orientation. We furthermore analyze the flow topology and show that the occurrence of chaotic advective mixing is controlled by the existence within the flow of transverse intersections between stable and unstable manifolds originating from the spheres. These insights are used to develop accurate predictions of the Lyapunov exponent distribution over possible flow orientations [2]. The difference of behavior observed for the SC and BCC lattices, which share the same symmetry point group, results from their different space group symmetries: a glide symmetry of the BCC lattice allows the occurrence of chaotic advection. These results point to a general theory of advective mixing and dispersion based upon the inherent symmetries of arbitrary crystalline structures.

References:

Click here to agree

Parallel 9-D / 621

Characterising multiphase flow functions with hysteresis from the mm to m scale in heterogeneous sandstones

Samuel Jackson¹; Sam Krevor¹

¹ Imperial College London

Corresponding Author(s): s.krevor@imperial.ac.uk

Incorporating sub-metre scale capillary pressure heterogeneity into upscaled numerical models is key to the successful prediction of low flow potential plume migration and trapping at the field scale. At low flow potential, nearing the capillary limit, the upscaled equivalent relative permeability incorporating capillary pressure heterogeneity is far from that derived at the viscous limit, dependent on the heterogeneity structure and flow rate, i.e. dependent on the capillary number.

To derive upscaled multiphase functions for field scale modelling, numerical or analytical methods are generally used either with statistical realisations of the permeability-capillary pressure field [3] or with simplified layered systems [4]. However, no protocol currently exists to efficiently derive these upscaled functions on heterogeneous rock cores directly from the subsurface, i.e. cores which
are truly representative of the system under consideration. Experimental observations must be combined with numerical upscaling so that subsurface rock cores can be directly characterised and used to accurately inform further modelling efforts.

In this work, we present a characterisation approach that incorporates experiments and numerical simulations to accurately characterise drainage and imbibition multiphase flow functions from the mm-m scale on heterogeneous subsurface rocks. We make use of a rich experimental core flood dataset obtained on N₂-DI water and CO₂-brine systems across multiple fractional flows, total flow rates and drainage-imbibition cycles. The experiments are performed on three distinct sandstones; a relative homogeneous Bentheimer outcrop core, a Bunter core from the Southern North Sea subsurface and a composite Captain core from the Northern North Sea subsurface.

Through characterisation of the mm scale capillary pressure heterogeneity and the viscous limit relative permeabilities we create parametrised 3D numerical rock cores. We build on the recent work of [5] and [6] by incorporating imbibition cycles into the characterisation approach, allowing the hysteretic nature of the systems to be analysed. The numerical cores are validated by simulating core flood experiments across a wide range of flow conditions, showing that mm-m scale experimental saturations and equivalent, low flow potential relative permeabilities can be accurately predicted for both drainage and imbibition cycles.

The numerical cores are then used to derive equivalent relative permeabilities across a wide range of conditions representative of flow regimes from the well to the far field in the subsurface, incorporating mm scale capillary pressure heterogeneities and saturation hysteresis. These functions show significant deviation from those derived in the viscous limit (orders of magnitude at some points), and highlight the impact that heterogeneity and hysteresis have on low potential fluid flow. We show that under this new approach, equivalent relative permeabilities can be effectively derived for drainage and imbibition cycles on heterogeneous rock cores, and that a relatively simple entry pressure scaling (or permeability-porosity scaling with the Leverett J-function) can be used to uniquely describe the capillary pressure heterogeneity with hysteresis.

References:
Click here to agree

Parallel 8-H / 130

Characterization of Rock Properties in Coupled Fluid Flow and Geomechanics Problems

Marcio Borges¹

¹ LNCC
Corresponding Author(s): marcio.rentes.borges@gmail.com

In the exploration of deep formations, alterations in pore pressure change the mechanical equilibrium of the porous medium leading to stress modifications which alter rock properties such as permeability and porosity and, consequently, the fluid flow pattern (Murad et al., 2013). The coupling of geomechanical effects and fluid flows is widely influenced by the natural rock heterogeneity (Mendes et al., 2012) and the predictability of computational models is limited by the availability of an adequate description of the formation properties, such as hydraulic conductivity, porosity, and poromechanical parameters. Since direct measurements of reservoir properties are only available at a small number of locations, the deterministic description of the hydraulic parameters cannot be accomplished at all relevant locations and alternative conceptualizations suggest that a stochastic methodology is indispensable to treat rock properties. In recent years the increase in field data acquisition (although in limited points) associated with the use of high performing computing have encouraged the use of dynamic data, such as well test data, historical pressure data, fractional flow rate, reservoir compaction and surface subsidence, directly in the simulation of processes in order to reduce uncertainties in rock properties and to improve the predictability of the models. In this work, we use the Markov-chain Monte Carlo (McMC) method to characterize the permeability, porosity and Young’s modulus fields in a two-phase problem coupled with the geomechanics of the adjacent rocks.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-F / 50

Characterization of dynamic fracture network extension in porous media by means of fractal geometry

Jianchao Cai¹ ; Shuyu Sun² ; Wei Wei¹ ; Yuxuan Xia¹

¹ China University of Geosciences (Wuhan)
² King Abdullah University of Science and Technology (KAUST)

Corresponding Author(s): caijc@cug.edu.cn

Fracture network can be commonly found or produced in many natural or damageable porous media, such as reservoirs, brittle materials and soil. Thus, fracture network and fractured porous media as well as their transport properties have received great attentions in many fields. Fractures are usually extended in length and aperture to form complex fracture network under some external conditions. The complexity of fracture network can be well quantitatively characterized by fractal geometry through fractal dimension and other parameters. Based on the improved box-counting technique, we measured the dynamic characterization of fracture network extension in porous media under drying process, and further respectively related fractal dimensions of fracture network to drying time, average aperture, moisture content and fracture porosity. It is found that the fractal dimension increases exponentially with drying time and average aperture, and decreases with moisture content in the form of power law. The transport capacity of fracture network is also related to the fractal dimension with drying time in the form of exponential function.

References:
3. T. Miao, S. Yang, Z. Long and B. Yu, Fractal analysis of permeability of dual-porosity media embe-
4. B. Li, R. Liu and Y. Jiang, A multiple fractal model for estimating permeability of dual-porosity
5. J. Liu, et al, Flow consistency between non-darcy flow in fracture network and nonlinear diffusion
   in matrix to gas production rate in fractured shale gas reservoirs, Transp. Porous Media, 111
   (2016) 97-121.
6. B. Noetinger, et al, Random walk methods for modeling hydrodynamic transport in porous and
8. A. Jafari and T. Babadagli, Estimation of equivalent fracture network permeability using fractal
10. P. Xu, C. Li, S. Qiu and A. P. Sasmito, A fractal netowk model for fractured porous media, Fractals,
    24 (2016) 1650018.
12. Y. Zhao, Z. Feng, Z. Lv, D. Zhao and W. Liang, Percolation laws of a fractal fracture-pore double
    medium, Fractals, 24 (2016) 1650053.
17. M. Vignes-Adler, A. Le Page and P. M. Adler, Fractal analysis of fracturing in two african regions,
    from satellite imagery to ground scale, Tectonophysics, 196 (1991) 69-86.
18. N. Matsumoto, K. Yomogida and S. Honda, Fractal analysis of fault systems in japan and the
19. A. Jafari and T. Babadagli, Effective fracture network permeability of geothermal reservoirs,
20. W. Wang, L. Kong, M. Zang and C. Zhang, Experimental research on crack extension and indoor
22. J. Cai, W. Wei, X. Hu, R. Liu, J Wang, Fractal characterization of dynamic fracture network exten-
    sion in porous media, Fractals 25 (2017) 1750023

Acceptance of Terms and Conditions:
Click here to agree
Characterization of modified nanoscale zero-valent iron particles transport through sandstones by nuclear magnetic resonance

Qian ZhangNone ; Yanhui DongNone

Corresponding Author(s): zhangqian@mail.igcas.ac.cn

With the increasing application of nanomaterials for environmental remediation, modified nanoscale zero-valent iron (nZVI) particles have been extensively examined in terms of their enhanced mobility in porous media as compared to bare nZVI particles. However, the monitoring of nZVI particle transport processes in low permeability media is still a challenge. To quantify the particle transport behavior, low-field nuclear magnetic resonance (LF-NMR) was employed to image the modified nZVI particles through tight artificial sandstones, which is preferable in the laboratory research of fluids in rock with the limited influence of internal gradients compared to high-field NMR. The spin-echo single point imaging (SE-SPI) sequence of NMR was applied to monitor the fluid flow processes in porous media in terms of the changing site-specific transverse relaxation time (T2), which was available to capture the transient effects at a time scale of seconds. More importantly, the SE-SPI sequence allows the high resolution detecting of nanoparticle transports through nanoscale porous materials. Quantitative concentration profiles converted from T2 distribution mapping profiles were analyzed by CXTFIT software to estimate the transport parameters. A comparison of the parameters calculated by various points along the length of the sandstone at different time intervals indicated that the dispersion coefficients, deposition rate constant, and collision efficiency decreased with time, whereas the fast deposition rate constant and average particle velocity increased with time. Meanwhile, the three-dimensional structure of sandstone, which was built using ORS Visual software with micro computed tomography (micro-CT) images, indicated the possibility of observing nanoparticles clogging in the pore throats. Accordingly, the modified nZVI particles exhibited better migration through porous media, which may result in their widespread commercial applications in the environment remediation.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 77

Characterizing CO2 Residual Trapping through Experiments

Author(s): Hailun Ni¹

Co-author(s): Charlotte Garing ¹ ; Sally Benson ¹

¹ Stanford University

Corresponding Author(s): hni@stanford.edu

CO2 storage in deep geologic formations is a necessary method to address the climate change problem. To ensure long-term security of the injected CO2, a better understanding of the post-injection CO2 residual trapping phenomena is needed. Using multiphase coreflooding experimental methods, we seek to characterize and predict the amount of CO2 residual trapping after injection.

Spatial heterogeneity is ubiquitous and exists from the pore scale to field scale. While large-scale heterogeneities have been much studied, small-scale heterogeneities received much less attention. However, it has recently been shown that millimeter-scale or small-scale heterogeneities have significant effects on large-scale CO2 injection (drainage) processes [3]. While some previous research has explored how small-scale heterogeneities affect the CO2 post-injection (imbibition) and trapping processes [2], [3], many uncertainties still remain about residual trapping. Historically, the dominant mechanism for residual trapping has been identified as snap-off trapping at the pore scale. However, recent studies have shown that capillary heterogeneity trapping at the millimeter scale can also be significant [4]. The relative importance of these two residual trapping mechanisms has not yet been established.
By conducting coreflooding experiments on sandstone samples with different degrees and nature of heterogeneity, we can investigate voxel-level trapping relationships, and gain insights into how small-scale heterogeneities affect CO2 residual trapping after capillary-dominated imbibition. The following conclusions can be drawn from the experimental results. Small-scale heterogeneities have less significant effects on imbibition than on drainage, as the CO2 saturation field is more uniform after imbibition. Although the effect of small-scale heterogeneities on imbibition may be less than for drainage, it is still significant. Within a core, voxel-level residual trapping correlates well with permeability and not porosity, demonstrating the influence of small-scale permeability change on the capillary-dominated imbibition process. Across different cores, core-averaged CO2 residual trapping efficiency is well correlated positively with the core-averaged degree of small-scale heterogeneity. By extrapolating that relationship, we can then quantify the contribution to residual trapping from the snap-off and the capillary heterogeneity trapping mechanism separately.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-D / 794

Characterizing porous media using experiments and image analysis via maximal inscribed spheres maps

Author(s): Rafael Salazar-Tio¹
Co-author(s): Emmanuel Toumelin ¹ ; Robert Mallan ¹ ; Mark Skalinski ¹ ; Paul Hart ¹

¹ Chevron

Corresponding Author(s): rswz@chevron.com

In this presentation, we explore applications of the maximal inscribed sphere (MIS) map to characterize porous media and show connections with other laboratory measurements. Three-dimensional maps can be computed from x-ray micro-tomography images of porous rocks and have been commonly used to simulate mercury injection capillary pressure (MICP) curves. We present additional applications of MIS maps to porous media characterization, that can be particularly useful in cases of heterogeneous multiscale pore systems.

A frequency distribution of the 3D MIS map can be used also as a definition of pore-size distribution, herein PSD-MIS. We discuss how drainage and imbibition hysteresis curves relate to the PSD-MIS curves. We also show a relationship between NMR and PSD-MIS; by tracking the actual location of the diffusing particles in NMR simulations, we found a clear correspondence between the T2 relaxation times classification and the PSD-MIS classification.

A relationship between 2D MIS-PSD and 3D MIS-PSD is presented, which enables the use of 2D images to estimate 3D MIS-PSD, allowing us, for instance, to take advantage of current SEM imaging technology that produces high resolution very large BSEM stitched images, and combine multiple scales of images to extend the size range from Nano scale to millimeter scale in the computed PSD-MIS. We show how the MIS tool complements MICP lab data for sizes above 100 microns, and gas adsorption lab data for sizes above 300 nanometers.

Finally, we introduce an adjustable 2D particle-particle separation method based on MIS. We apply this method to estimate grain size distributions that are compared with similar results from laser particle analysis. Another application addresses the estimation of MICP curves from 2D images. Based on the diversity of applications of MIS maps presented here, we conclude by discussing...
Parallel 4-C / 350

Collapse of chemically altered porous surface decreases fracture permeability, frictional strength and stability

Kasparas Spokas\textsuperscript{1} ; Yi Fang\textsuperscript{2} ; Jeffrey P. Fitts\textsuperscript{1} ; Catherine A. Peters\textsuperscript{1} ; Derek Elsworth\textsuperscript{2}

\textsuperscript{1} Princeton University
\textsuperscript{2} Pennsylvania State University

Corresponding Author(s): kspokas@princeton.edu

In many subsurface energy activities, such as hydraulic fracturing, geologic carbon storage, deep well disposal, and geothermal energy, the injection or extraction of fluids results in significant mechanical and chemical perturbations. These perturbations pose risks in promoting unwanted fluid leakage pathways, such as faults and fractures, through chemical reactions and mechanical failure. The flow of reactive fluids through fractures has been shown to dissolve reactive minerals and thereby increase permeability. However, it remains unclear how this dissolution influences the frictional properties of fractures and how the altered fractures behave during shear rupture. To properly assess the risks associated with subsurface energy activities, this study experimentally investigates how mineral dissolution on fracture surfaces affect fracture flow and frictional properties under stress.

Experiments were performed using 1.5-inch long saw-cut rock fractures from the Eagle Ford formation, a calcite-rich laminated shale. Experiments were performed in two stages: reactive fluid flow experiments and tri-axial shearing experiments. During the first stage, samples were organized into two sets, where one set was exposed to an acidic brine and the other exposed to a near-neutral brine. After flow, X-ray computed tomographic imaging showed the formation of a highly porous altered layer for samples exposed to the acidic brine, and no significant alteration for samples exposed to the near-neutral brine. This altered layer is created primarily from the dissolution of calcite grains, leaving a porous intact matrix of non-reactive minerals at the fracture surface. During the second stage, samples were sheared in a tri-axial testing apparatus that independently supplied confining pressure and differential pore pressure along the fracture length at prescribed sliding velocities, independently measuring friction and permeability. Samples were confined to 3 MPa effective stress with shear velocity down- and up-steps of 1 um/s and 10 um/s.

X-ray computed tomographic imaging following the shearing experiments revealed that the porous altered fracture surface layers had collapsed into a layer of fine particles that filled the fracture aperture, effectively sealing the fracture. This is confirmed by permeability measurements during the initial compaction in the shearing apparatus, where the permeability of samples with an altered surface layer decreased one order of magnitude lower than the samples without an altered layer. This difference in permeability between the sample sets persisted through the entire shearing experiments. Results from the shearing experiments show that the altered sample set exhibited both lower frictional strength and stability. This is because for the samples exposed to non-reactive brine, the micro-roughness at the fracture interface results in interlocking micro-asperities that both increase the fracture strength and stability. For the altered samples, however, the layer of fine grained particles filling the aperture separate the two fracture walls, preventing the formation of interlocking micro-asperities. As a result, we describe the fracture surfaces as “surfing” on the layer of fine-grained particles.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-A / 46

Colloid-facilitated radionuclide transport through a bead-packed column and direct simulation using lattice-Boltzmann and random walk particle tracking

Jae Kyoung Cho¹ ; Xiaolong Yin¹ ; Keith B. Neeves¹ ; Ning Wu¹ ; Kenton Rod² ; Wooyong Um² ; Jaehun Chun²

¹ Colorado School of Mines
² Pacific Northwest National Laboratory

Corresponding Author(s): xyin@mines.edu

It is well known that the radionuclide-carrying colloids in ground water can facilitate the transport of contaminants in the subsurface. A set of column experiments under physically and chemically heterogeneous conditions was conducted. Pore velocity was maintained below 100 cm/d and solution of CsI and silica colloids (1 micron diameter) was injected through saturated columns. At the same time, pore-scale simulation using lattice Boltzmann (LB) and random-walk particle tracking (RWPT) was used to solve the advection-diffusion equation (ADE) to match the breakthrough curves and dispersion coefficients of column experiment. With high-performance computing, we directly simulated flow and convective transport of non-adsorbing and adsorbing colloids in the entire column (L = 10.3 cm, D = 0.75 cm, resolved by 169 × 169 × 1722 voxels). We compared not only the dispersion coefficients, but also the breakthrough curves between column experiments and pore-scale simulations for the first time. The latter comparison was enabled by an algorithm that effectively maintained load balance and parallel efficiency.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-A / 357

Colloidal transport in a microfluidic porous medium with surface charge heterogeneity

Author(s): Yang Guo¹
Co-author(s): JaeKyoung Cho¹ ; Keith B. Neeves¹ ; Ning Wu¹ ; Xiaolong Yin¹

¹ Colorado School of Mines

Corresponding Author(s): yguo@mines.edu

Colloidal facilitated transport of contaminants is a major concern for transport of low solubility chemicals in ground water flows. Compared with themselves alone, contaminants travel much further after adsorbing to natural colloidal particles, as far as kilometers over years. Therefore, understanding the transport behavior of colloids would provide insightful knowledge for environmental protection and remedy. In the past most lab-scale experiments focused on studying the interactions between particles and homogeneous or physically heterogeneous porous media. In reality, porous media exhibit different chemical properties at the grain scale. To shed some light in this aspect, we built a family of pseudo-three-dimensional microfluidic porous media models packed by 10 μm polystyrene (PS) beads with opposite surface charges. Each porous medium contains more than 6000
beads and has a size of 1000 µm in length, 600 µm in width and 15 µm in height. An on-chip cross channel linked with an off-chip 4-way valve was applied to generate a step input of concentrated colloidal suspension, which also greatly reduced the influence of Taylor dispersion of colloidal particles. We further studied the effect of chemical heterogeneity on the transport and retention of colloidal particles. The breakthrough of the particles was recorded at the downstream of the porous medium. The colloidal retention profile was mapped using a confocal microscope. Beads with different surface properties are distinguished by their different fluorescent labels. Therefore we also obtained colloidal retention data for beads with different surface properties. With our platform, we developed a correlation between the overall collector efficiency and its constitutive collector efficiency under different salt conditions.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 629

Combined wicking and drying of a NaCl solution in porous media as studied by NMR

Leo Pel1 ; Raheleh Pishkari1 ; Olaf Adan1

1 Eindhoven University of Technology

Corresponding Author(s): l.pel@tue.nl

Salt are a major cause of destruction by crystallization of porous media. Salt will in general enter a porous medium by advection with moisture or diffusion within the moisture. A special situation which occurs often in marine environments in which case there is a permanent supply of sea water at one side of a porous material such as a concrete structure. At the other side, the structure is exposed to continuous drying in the open air. In such a case there will be a mixed situation for describing the transport. Evaporation from the air exposed side provides a continuous moisture sink which is compensated by capillary suction, i.e., wicking, of the sea water. As a result there will be a continuous flux of NaCl ions to the surface. As a result of this combined process the NaCl concentration at the drying surface will increase slowly until crystallization starts. Using a specially designed Nuclear Magnetic Resonance (NMR) setup, the 1H, 23Na and 35Cl content can measured quasi-simultaneously. Hence this NMR method gives us the possibility for real-time monitoring of transport processes of the ions during experiments. We have measured the transport of the both Na and Cl during this combined process for both a sandstone and concrete. The results can be described by a simple analytic model which indicates the concentration profiles can be described an exponential decay.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 947

Combining Products of Fossil Energy R&D with Advanced Data Computing to Develop a Virtual Subsurface Data Framework for the U.S.

Rose Kelly1 ; Devin Justman2 ; Baker D.V. "Vic"3 ; Bauer Jennifer4 ; Dehlin Mark3 ; Jones T.J.3 ; Rowan Chad4 ; Digiulio Jennifer5 ; Sabbatino Michael6
Data has been described as the world’s new oil, as a resource with immense potential to inform and transform daily life as well as science and engineering. The volume of newly generated scientific data is projected to exceed 40,000 exabytes by 2020. At present, however, only 20% of the world’s data are preserved online. Field, lab, and computing datasets all contribute to an improved understanding of subsurface systems. Within the United States (U.S.) Department of Energy (DOE), research to constrain and predict subsurface behavior spans oil and gas, carbon storage, groundwater, geothermal and underground waste disposal portfolios. Beyond DOE, studies of U.S. subsurface systems have contributed to a growing but disparate knowledge base of the in situ geology and pore filling media at a range of scales and resolutions.

To support energy research and development, we are using a combination of open-source and custom developed advanced computing capabilities to facilitate development of a virtual subsurface data framework for the U.S. This framework requires the integration of research, scientific, and engineering data resources, including subsurface characterization, modeling, and analytical datasets. However, subsurface datasets are still challenging to access, discontinuous in scale, and variable in resolution, but the proliferation of online data and improved curation of DOE Fossil Energy (FE) research products, there are significant opportunities to advance access and knowledge of subsurface systems. NETL’s Energy Data xChange (EDX) is an online platform designed to address research data needs by improving access to energy R&D products through advanced search and access capabilities and hosts private, virtualized trust communities to support more efficient and effective, multi-organizational R&D.

Through the private and public side of EDX, NETL researchers are assembling and hosting structured and unstructured data and resources related to the subsurface U.S. These resources are being integrated with those curated from DOE and open-sources. The EDX team has also implemented a big data, machine learning custom SmartSearch tool to help locate and source data from the whole of the worldwide web. This tool is currently in beta testing, but has been used, along with custom data integration and database generation scripts, to produce a database of open, global oil and gas infrastructure resources that is being paired with the virtual subsurface data catalog. All of these resources will be hosted in EDX through its standard search capabilities, but are also being implemented in EDX’s web-mapping tool, Geocube. Geocube allows users to visualize surface and subsurface spatial datasets, add their own datasets to the visualization, and download resources if desired. Ultimately, EDX’s public-private capabilities seek to facilitate more effective research for subsurface scientists and increasingly pairs EDX hosted resources with other online capabilities, data, custom machine learning algorithms and capabilities to enhance user experience, and provide research teams with the resources needed to make subsurface energy research more efficient, reduce redundancy, and drive innovation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-G / 708

Comparative Study on Nano-scale Pore Heterogeneities of Marine and Lacustrine Shales by Multifractal analysis

Author(s): Xiaofei Hu¹
Co-author(s): Hucheng Deng ¹; Zhehui Jin ²

¹ ¹, College of Energy, Chengdu University of Technology. 2, School of Mining and Petroleum Engineering, Faculty of Engineering, University of Alberta.
The heterogeneous nano-scale pore structures have a significant effect on hydrocarbon properties and matrix mechanics in shale. Marine and lacustrine shales may have varying pore structures due to different depositional settings. Understanding the nano-scale pore structures in marine and lacustrine shales can provide important insights into fractal geometry theory. Therefore, we use the low-pressure nitrogen adsorption and new visual method of multi-scale field emission scanning electron microscopy (FESEM) to measure the geochemical and petrological characteristics of marine and lacustrine shale cores. Based on the fractal and multifractal analysis to study pore heterogeneities, we explicitly investigate the shale microstructures, including irregularities and distributions and their relations to transport phenomena.

In this work, we collect 32 lacustrine shale samples from Lower Jurassic Formation and 10 marine shale samples from Longmaxi Formation of Sichuan Basin in China. We carry out the spatial fractal analysis by nitrogen adsorption with Frenkel-Halsey-Hill (FHH) model, which has been widely applied in the characterization of the pore size distributions and properties. And use visible multi-scale FESEM images to investigate pore heterogeneities by multifractal analysis. The results of low-pressure nitrogen adsorption with FHH model show that all samples, adsorption fractal dimensions can be classified into two regions based on fractal dimensions D1 and D2, corresponding to large pores and small pores, respectively. For both marine and lacustrine shales, D1 is generally larger than D2, indicating the weaker heterogeneity in small pore structures. Meanwhile, The fractal dimension D1 and D2 of lacustrine shale are generally lower than that of marine shale, indicating smaller heterogeneity in lacustrine shale, due to lower maturity and fewer organic pores. Based on the features of multifractal spectrum curves, the results of the multifractal analysis show that the heterogeneities of lacustrine shale are generally lower than that of marine shale, which is the same as the FHH model. Meanwhile, the three multifractal parameters of multifractal spectrum curves depicted that the heterogeneities closely related to the shale composition, organic matter properties, and geophysical characteristics. The multifractal parameters of marine shale are generally larger than lacustrine shale, indicating that marine shale pore structures are more complicated. Compared with results of FHH model by nitrogen adsorption, the results of multifractal analysis by multi-scale FESEM could provide more accurate information on the heterogeneity properties of shale samples. The measurements of petrophysical and geochemistry properties are closely associated and multifractal parameters. In addition, the quantitative analysis of multifractal parameters is in agreement with the field research, which is important for the evaluation of oil and gas flow system in shale.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-B / 869

Comparative simulation of reactive flow in catalytic filter using 3D pore-scale model on CT image and 1D effective model

Robert Greiner1 ; Torben Prill2 ; Oleg Illiev3 ; B. van Setten4 ; Martin Votsmeier5
In order to improve the performance of the exhaust after treatment system and keep reasonable complexity, the number of the used devices is reduced by enhancing wall flow particulate filters with a catalytic functionality, like selective catalytic reduction in diesel or three way catalysis in gasoline vehicles. In this case the solid matrix of the filtering media consists from inert grains and active grains. For the simulation of such devices, effective 1D models are regularly used, because they are relatively simple and fast in comparison to higher dimensional models, while reproducing most of the experimentally observed phenomena with sufficient accuracy. The reduction of the complexity in the modeling, however, is achieved by introducing many simplifying assumptions.

As it will be seen in this presentation, 1D models do not always reproduce detailed 3D simulations. Here we compare a standard 1D homogenous wall model with a 3D pore-scale model. The latter describes convection and diffusion in the pores and in washcoat grains, and absorption in the washcoat grains. In fact, washcoat particles are nanoporous and surface reaction (adsorption) occurs at this scale. Software tool called PoreChem has been used for simulating the reactive flow at pore scale. A wall segment of a real particulate filter was used in the simulation. The three-dimensional structure of the wall segment was obtained by X-ray microtomography, in which we resolved the different materials: Pores, (inert) Substrate and (active) Washcoat. A first order reaction was studied to examine if 1D simulations based on effective (Darcy scale) model can describe the behavior of a catalytic filter wall sufficiently well. In simulations the adsorption rate constant varied while the other properties, like temperature and flow speed remained constant. The conversion (adsorbed amount) was computed for different reaction rate. The discrepancy between the results obtained with the 3D and 1D models increase with higher reaction rates. They are caused by the inhomogeneous flow and washcoat distribution in the 3D system that cannot be described well with a homogenized 1D model. 3D models are therefore useful to optimize the microstructure of catalytic particulate filters.

References:


Click here to agree

Poster 2 / 197

Comparison of Model Approaches for Gas Transport in Compacted Bentonite: A Current Task in the International DECOVALEX Project

Author(s): Jens Birkholzer

Co-author(s): Jonny Rutqvist; Kunhwi Kim

Corresponding Author(s): jtbirkholzer@lbl.gov

The DECOVALEX project is an international research and model comparison collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical (THM) processes in geological systems. Prediction of these coupled effects is an essential part of the safety assessment of geologic disposal systems for radioactive waste and spent nuclear fuel, but also for a range of other sub-surface engineering activities such as carbon dioxide subsurface storage, enhanced geothermal systems, and unconventional oil and gas production through hydraulic fracturing. DECOVALEX involves analysis and comparative modeling of state-of-the-art laboratory and field experiments, with
various international research teams providing a wide range of perspectives and solutions to these complex problems.

One of the analysis and modeling tasks of the current DECOVALEX phase centers on the transport of gas through low-permeability clay-based materials such as bentonite or argillite rock. In a geological repository for radioactive waste, the corrosion of the ferrous materials, radioactive decay of the waste, radiolysis of organic materials and water, and the microbial breakdown of organic materials will produce gas, the most important of which (by volume) is hydrogen. As gas is produced, it will initially accumulate until gas pressure is eventually high enough to drive gas away from its source. Understanding the long-term fate of such gas transport and its impact on the surrounding materials is therefore important in the development of a geological disposal facility for radioactive waste.

Research teams involved in the modeling task use a range of different approaches to simulate gas transport data from a series of well-controlled laboratory tests, in a staged manner building in complexity (both in terms of the experimental and modelling approaches). Special attention is given to the THM mechanisms controlling factors for initiation and evolution of gas flow, such as gas entry, mechanical damage, pathway dilation and flow, as well as pathway stability and sealing, all of which will impact barrier performance. This presentation will provide an overview of process understanding and model approaches, and then will discuss in more details two specific numerical models to analyze gas-migration laboratory experiments on mechanically confined bentonite samples. The first model is a continuum model based on multiphase fluid flow, linear poro-elasticity and moisture swelling, with gas permeability related to the minimum effective compressive stress. The second model is a discrete fracture model based on continuum multiphase fluid flow linked with a lattice model to represent discrete fracture developments. In the continuum model, the key to capture observed responses is the stress-dependent gas permeability and moisture shrinkage. In the discontinuum model, the key processes involved are shear failure creating a dense discrete fracture network and abrupt permeability enhancement. Both models capture reasonable well the measured evolution of gas flow, pressure and stress, including the abrupt responses observed once an apparent threshold gas pressure is exceeded. Further modeling of other experiments conducted on the same type of bentonite (e.g. spherical flow versus linear flow) will be necessary to better distinguish between different underlying and controlling processes occurring within the sample.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 688

Comparison of Types of Nanoscale Heterogeneity on Colloid Retention and Release at Interfaces

Scott Bradford\textsuperscript{1} ; Hyunjung Kim\textsuperscript{2} ; Chongyang Shen\textsuperscript{3} ; Salini Sasidharan\textsuperscript{4} ; Hwang Gukhwa\textsuperscript{5}

\textsuperscript{1} USDA ARS
\textsuperscript{2} Department of Mineral Resources and Energy Engineering
\textsuperscript{3} China Agricultural University
\textsuperscript{4} Department of Environmental Sciences

Corresponding Author(s): scott.bradford@ars.usda.gov

Nanoscale roughness (NR) is a physical heterogeneity on all surfaces, whereas chemical heterogeneity (CH) may sometimes arise from spatial variability in charge (CH1), Hamaker constant (CH2), and contact angles (CH3). Expressions were developed to determine the mean interaction energy between a colloid and a solid-water interface, or another colloid, when both surfaces contain binary NR and CH1 or CH2 or CH3. All of these interaction energy relations considered double layer, van der Waals, Lewis acid-base, and Born interactions. The influence of nanoscale roughness and CH parameters, solution ionic strength (IS), and colloid size on predicted interaction energy profiles was then investigated. CH tended to reduce the energy barrier and create deeper primary minima on net
electrostatically unfavorable surfaces. However, the role of CH was always greatest on smooth surfaces with larger amounts of CH, especially for smaller colloids and higher IS. Furthermore, CH3 was predicted to have a larger influence on colloid retention and release than CH1 or CH2. However, predicted interaction energy profiles were demonstrated to be mainly dominated by NR, which tended to lower the energy barrier height and the depths of both the secondary and primary minima, especially when the roughness fraction was small. This dramatically increased the relative importance of primary to secondary minima interactions on net electrostatically unfavorable surfaces, especially when roughness occurred on both surfaces and for conditions that produced small energy barriers on smooth surfaces. Energy balance calculations indicate that the combined influence of roughness and Born repulsion produced a shallow primary minimum that was susceptible to diffusive or hydrodynamic removal, even in the presence of significant amounts of CH.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-C / 109

Comparison of sequential and fully-coupled approaches for flow and geomechanics

Author(s): Martin Beck

Co-author(s): Holger Class

University of Stuttgart

Corresponding Author(s): martin.beck@iws.uni-stuttgart.de

Choosing an appropriate modelling approach for fluid flow and stress field interaction in rocks belongs to the key problems within the context of several subsurface applications such as geothermal power generation, disposal of waste water, CO2 storage or hydraulic fracturing. A central issue in this respect is the question of whether the equations for flow and geomechanics are solved in a fully-coupled manner or by using an operator splitting or a sequential scheme. The latter is a common choice to link existing codes for flow and mechanics. We present a concept that has both implementations available to allow for a detailed comparison. Following this, we introduce a sequential so-called ‘fixed-stress’ scheme after Kim et al. (2010) and a fully-coupled multi-phase flow and geomechanics approach. Both are implemented in the open-source simulation toolbox DuMuX. We test the schemes on a realistic hydraulic fracturing scenario which examines the potential reactivation of a fault due to injection-induced changes of the pressure and stress field. This allows us to examine the applicability of our implemented approaches and, at the same time, provides us with a validity check of our results, as this scenario was previously studied by Rutqvist et al. (2013) using a sequential coupling of TOUGH2 and FLAC3D. Having a fully-coupled scheme at hand also enables us to compare the convergence behaviour and the computational effort of the different coupling schemes. While performing this, we gained insights in how to tackle the high non-linearity of the problem. Furthermore, the high dependence of the solution on the number of iterations performed for the sequential scheme is a key finding of this study.

References:


Acceptance of Terms and Conditions:
Click here to agree
Poster 4 / 462

Compositional two-phase fluid flow in porous media: from the pore scale to Darcy’s scale

Shuyu Sun

1 King Abdullah University of Science and Technology (KAUST)

Corresponding Author(s): shuyu.sun@kaust.edu.sa

Compositional two-phase fluid flow in porous media, especially on geometrically complex domains, require high fidelity geometric discretization. Moreover, since multi-component multi-phase flow and transport in porous media usually come with strong nonlinearity and stiffness in multiple spatial and temporal scales, it is necessary to deploy a multi-scale approach that is inevitably memory-intensive and time-consuming, requiring robust and high-accurate algorithms as well as high-performance computing infrastructure. We present an overview of recent advances in simulations of multi-component two-phase fluid flow in porous media at Darcy’s scale and at the pore scale as well as their coupling. We discuss the modeling and computational techniques for both conventional and unconventional petroleum reservoirs, in particular the non-Darcy flow in tight geological formation.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-H / 626

Computer simulation of the geometric pore size and validation with glass bead tests for metal wire meshes

Andreas Wiegmann1 ; Sven Linden2 ; Erik Glatt1

1 Math2Market
2 Math2Market GmbH

Corresponding Author(s): andreas.wiegmann@math2market.de

Metal wire mesh is used in a wide variety of filtration applications. The geometric pore size is the diameter of the largest spherical bead that can pass through such a mesh. It is a very important quality measure and is found by filtering spherical glass beads with the mesh. Here, we describe how the geometric pore size of a mesh can be reproduced by computer simulations with GeoDict. The simulation works based on 3d voxelized models of the mesh. The 3d models can be obtained in two ways. The first way is taking µCT scans of existing mesh. The second way is creating purely virtual geometric models of next generation metal wire mesh with GeoDict’s WeaveGeo module.

The geometric pore size is simulated by tracing spheres through the pores in the model using Saito’s fast Euclidean distance transform and Dijkstra’s fast marching algorithm. It turns out that the surprisingly good agreement between simulations of the geometric pore size and measurements with glass beads is due to the fortuitous cancellation of two errors in the simulation. In contrast, for a good representation of the center line of the through-pore, one needs to avoid one of these errors.

References:

Parallel 11-D / 162

Condensation, Imbibition and Crystallization of Molecular Liquids in Nanoporous Solids

Kathrin Sentker¹ ; Mark Busch¹ ; Patrick Huber¹

¹ Hamburg University of Technology

Corresponding Author(s): patrick.huber@tuhh.de

Vapor-condensation and capillarity-driven, spontaneous imbibition allow one to fill nanoporous media in a controlled manner with molecular liquids. We present experimental studies on the dynamics of these filling processes for a variety of porous media (silicon, silica, and gold with pore diameters ranging from 2 to 100 nm). These experiments are aimed at an exploration of the rheology of nanoconfined liquids as a function of the complexity of their building blocks (hydrocarbons, liquid crystals, and water) (1,2,3). Temperature-dependent X-ray and neutron diffraction studies complement these non-equilibrium with equilibrium studies on the thermodynamics of the confined liquids, encompassing suppressed phase transitions (1), extremely supercooled (1,4) and textured crystalline states (4) as well as entirely new liquid crystalline phases (5).

References:


Click here to agree

Parallel 8-B / 638

Conjugate soil-vegetation-air-radiation model for studying the environmental impact of porous media such as vegetation

Lento Manickathan¹ ; Aytaç Kubilay² ; Thijs Defraeye² ; Jonas Allegrini² ; Dominique Derome² ; Jan Carmeliet¹

¹ ETHZ
² Empa

Corresponding Author(s): cajan@ethz.ch
In this paper, a conjugate model is presented to evaluate the effect of vegetation on the surrounding environment. Vegetation intercepts solar radiation, providing shading to the ground, and offers natural cooling through evapotranspiration, cooling the air flowing through the vegetation. However, vegetation also slows down the air flow and its transpirative cooling potential is strongly dependent on the water availability in the soil. In order to accurately account for all these phenomena, the vegetation model should include airflow including momentum, heat, moisture, radiation and the water cycle in an integrated approach.

Vegetation, in this study a tree, is modeled as porous medium, including source/sink terms for heat, mass and momentum fluxes. A radiation model is developed to model the short-wave and long-wave radiative heat fluxes between the leaf surfaces and the surrounding environment as well as the extinction of radiation passing through the porous medium. The radiation model enables to model in detail the impact of the diurnal variations of solar intensity and direction, and the long-wave radiative fluxes between vegetation and nearby surfaces. A finite volume approach is applied to the discretization of the vegetation foliage where the leaves of the tree are aggregated into finite volumes. The heat and mass exchanges are determined from a leaf energy balance model applied foreeach leave in the discrete volume. This enables a description of the heat and mass fluxes from vegetation with a realistic geometry and leaf density distribution. Furthermore, the transpiration process at the leaf surfaces is coupled to the water availability at the roots of the plants. For this, a full water cycle model for vegetation or conjugate soil-vegetation-air-radiation model is developed. The vegetation-air model is coupled with a soil model to capture the full water cycle. The vegetation is characterized in the soil using a root area density (RAD) distribution function, which provides sink terms of water uptake by the roots in the soil. The soil water transport model is coupled with the evapotranspiration at the leaves, taking into account the water transport within the tree.

In the present study, the influence of trees on the local climate in cities is studied using the developed vegetation model implemented in OpenFOAM. As an example, we quantify the influence of shading and transpirative cooling due to vegetation on pedestrian thermal comfort inside a street canyon. The influence of various tree features such as size, shape, location and quantity is studied. The transpirative cooling effect of a tree is found to be highest at lower wind speed and diminishes in humid and low temperature conditions, where the vapor pressure of air is near saturation and the transpiration from vegetation diminishes. The transpirative cooling effect of vegetation depends primarily on its leaf area density due to the coupled effect on both wind speed and air temperature. If vegetation does not transpire, increasing the number of trees results in an increase in air temperature downstream of the vegetation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 555

Constitutive Relations for a New Theoretical Framework Describing 2-Phase-Flow in Porous Media

Author(s): Mathias Winkler

Co-author(s): Magnus Aa. Gjennestad \(^1\); Alex Hansen \(^2\); Santanu Sinha \(^3\)

\(^1\) Norwegian University of Science & Technology
\(^2\) Norwegian University of Science and Technology
\(^3\) NTNU

Corresponding Author(s): mathias.winkler@ntnu.no

Recently, a new theoretical framework to describe 2-phase flow in porous media has been put forward by our research group. Within this theory, a transport equation for the wetting phase saturation can be derived. In order to utilize this new theory a constitutive relation is needed that
characterizes the “mixing” of the two fluids. Here mixing is understood not as mixing on a molecular level, but rather as the mixing of the two fluids seen on a meso- or macroscopic scale. In this contribution, we use constitutive relations obtained from mesoscale network models and apply the new theory to transient states on the macroscale.

References:

Acceptance of Terms and Conditions:
Click here to agree

---

Poster 3 / 840

Contact Angle Measurement and Molecular Dynamics Simulation of Wettability Alteration on Calcite Surface

Author(s): Hongna Ding

Co-author(s): Sheik Rahman

Corresponding Author(s): hongnading1989@hotmail.com

This study describes wettability alteration mechanism of calcite surface by low salinity water (diluted seawater) and ion tuned water (regarding to potential determining ions, PDI). The contact angles of brine droplets on calcite surfaces that immersed in oil were measured. The relative ability in modifying the surface wettability of these three ion species (Ca$^{2+}$, Mg$^{2+}$ and SO$^{42-}$ ions) thus is evaluated. Contact angles results suggested that 10 times diluted seawater is sufficient to alter the calcite surface into more water-wet. In addition, increasing SO$^{42-}$ and Mg$^{2+}$ concentration whilst decreasing Ca$^{2+}$ concentration modify the calcite into more water-wet. Therefore, an ion tuned water which is obtained by manipulating seawater to contain four times SO$^{42-}$ concentration, two times Mg$^{2+}$ concentration and one-half Ca$^{2+}$ concentration gives rise to a maximum magnitude of water wetness of calcite surface. Moreover, molecular dynamics (MD) simulation of contact angles has been carried out in order to gain more fundamental understanding on the relationship between wettability and salinity or PDI effect. MD simulation results suggested that SO$^{42-}$ and Mg$^{2+}$ ions tend to incorporate into calcite lattice and disturb the orientation of water molecules at interface. In general, MD showed a good consistent with experimental results. Therefore, this paper is expected to provide some new insights into low salinity water flooding and ion tuned water flooding in carbonate reservoirs.

References:

Acceptance of Terms and Conditions:
Click here to agree

---

Poster 1 / 254

Contact Angle Measurements of scCO2 and Brine in 3D Printed Models with Varying Surface Roughness

Author(s): Laura Dalton

Co-author(s): Dustin Crandall $^1$; Angela Goodman $^1$

$^1$ U.S. Department of Energy National Energy Technology Laboratory

Corresponding Author(s): laura.dalton@netl.doe.gov

Geometric material pore networks are highly tortuous with intricate geometries and varying surface roughness. It is reported in literature that both pore geometry and surface roughness influence flow
through porous media (Ketcham and Carlson, 2001; Noiriel et al., 2016; Lv et al., 2017). Surface roughness is quantified by the deviations in the direction of flow perpendicular to the real surface. Simplified pore networks with known geometric shapes and the quantified surface roughness affords the opportunity to back-calculate internal forces and begin to quantify the effect on contact angles. 3D printed models printed using acrylonitrile butadiene styrene were designed with an internal structure of void geometries to represent a flow path with different geometric interfaces. To look at surface roughness, different techniques were used to add surface roughness to the models. The models were exposed to chemicals that reacted with the material surface to add microscopic surface roughness and macroscopic roughness was added via design and printing techniques. Each model was placed in a core flooding setup and exposed to a series of CO2-saturated brine and scCO2 injections to mimic underground conditions. Once at residual conditions, the core-flooding setup was set to shut-in conditions and scanned used X-Ray micro-computed tomography. 3D reconstructions contain information to measure contact angles, analyze forces, and correlate each to the geometries and surface roughness of each model. Analysis of the local impact to scCO2-brine contact angles within pores with varying surface roughness will be presented.

References:

Parallel 11-G / 637

Continuum modeling of porous media based on pore-space accessibility

Zongyu Gu1; Martin Bazant1

1 MIT

Corresponding Author(s): zygu@mit.edu

In continuum modeling of porous media, it is necessary to characterize microscopic features of the pore space using a small set of continuum-scale parameters, such as porosity, tortuosity, etc., which are then linked to transport coefficients or other macroscopic properties. For phenomena that depend on the physical dimensions of pores, the pore-size distribution is also commonly used. It is well-known that the pore-size distribution alone is not sufficient for predicting continuum-level, often multiphase, processes when the connectivity of different sized pores also plays an important role. We propose a new continuum-scale parameter – the "accessibility" ($\alpha$), to describe the network connectivity of different sized pores. Small accessibility ($\alpha \to 0$) favors serial connection between different sized pores, while large accessibility ($\alpha \to 1$) favors parallel arrangement; the model of bundle of straight capillaries corresponds to the latter. Defined based on a probabilistic framework, $\alpha$ has a number of interesting physical interpretations, and can be related to concepts in queueing theory. We show that the accessibility concept provides a useful first approximation to connectivity effects in porous media, which serve to improve simple models previously derived based on the bundle model, and has broader utility in continuum modeling in more general settings.

References:
Acceptance of Terms and Conditions: 

Parallel 11-A / 223
Contribution of Heterogeneity within Semi-Confining Shale Layers to Mixing and Storage of Dissolved CO2

Author(s): Elif Agartan¹
Co-author(s): Tissa Illangasekare ¹; Javier Vargas-Johnson ¹; Abdullah Cihan ²; Jens T. Birkholzer ²

¹ Colorado School of Mines
² Lawrence Berkeley National Laboratory

Corresponding Author(s): elif.agartan@gmail.com

Dissolution trapping is one of the mechanisms that contributes to stable storage of carbon dioxide (CO2) in deep geologic formations with brine. Basic to the process is the supercritical CO2 (scCO2) dissolving in the formation brine and the subsequent mixing of dissolved CO2 and brine in the deeper zones of the formation. In most conceptual models, it is assumed that the mixing is controlled by convection of the heavier solute moving vertically as unstable fingers. In our previous work, we have shown that presence of heterogeneity in the formation disrupts the convective fingers and thus affecting the effective mixing rates. In one of our previous studies that used field-scale modeling, we highlighted two key mechanisms, i.e. convective mixing and diffusion controlled trapping, contributing to dissolution trapping in multilayered systems with homogeneous low-permeability layers (e.g. shales). However, these low-permeability layers are not always homogeneous due to their composition and texture variations in addition to the presence of faults, fractures and fissures. The purpose of this study is to investigate the potential outcomes of heterogeneity present within these semi-confining low-permeability layers in regards to mixing and storage of dissolved CO2. An intermediate-scale laboratory experiment representing a multilayer system with a heterogeneous low-permeability layer was designed to investigate the contribution of convective mixing, diffusion controlled trapping and back diffusion to long-term storage of dissolved CO2. The experiment was performed using a surrogate fluid combination, NaBr solution and water, to represent dissolved CO2 and brine, respectively, under ambient pressure and temperature conditions. In order to investigate the observed mechanisms in detail for the different distributions of the same low-permeability materials having similar volume ratios with the experimentally studied scenario, first the numerical model was verified with the experimental results. Then, several heterogeneous low-permeability layer scenarios were tested numerically. The experimental and modeling results showed that connectivity of higher permeability material within the semi-confining low-permeability layers contributes to mixing through brine leakage between upper and lower aquifers, storage through diffusion, and in the long term, back diffusion of stored mass due to reversed concentration gradients.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-A / 329

Control of carbon dioxide convective dissolution with chemical reactions in porous media: Enhanced dissolution flux

Laurence Rongy¹; Vanessa Loodts¹; Carelle Thomas¹; Hind Saghou¹; Bernard Knaepen¹; Anne De Wit¹

¹ Universite libre de Bruxelles (ULB)

Corresponding Author(s): lrongy@ulb.ac.be

Dissolution-driven convection in partially miscible systems has regained much interest in the context of CO2 sequestration [1]. A buoyantly unstable density stratification can build upon dissolution of CO2 into brine, thereby driving convection. Dissolution and convection are known to improve the safety of the sequestration process by reducing the risks of leaks of CO2 to the atmosphere. The temporal evolution of dissolution-driven convective dynamics has been characterized in detail and it has been shown that the dissolution flux reaches a steady-state value before shutdown [2]. The
question remains, however, as to how the efficiency of such process depends on the chemical properties of the storage site and how chemical reactions can affect the steady-state fluxes. Reactions can indeed accelerate or slow down the development of dissolution-driven convection in partially miscible stratifications when they impact the density profile in the host fluid phase. The different possible dynamics taking place during the convective dissolution of CO$_2$ into a host fluid containing a dissolved reactant B have been classified for a chemical reaction CO$_2$ + B $\rightarrow$ C (product), assuming that all species diffuse at the same rate [3,4]. We now consider the more general case where solutes can diffuse at different rates. Using nonlinear simulations, we show that depending on the type of density profile developing in the host fluid, one or two convection zones can be observed. Although changing the diffusivity ratios can have non-trivial effects, decreasing the diffusion coefficient of product C or increasing the diffusion coefficient of reactant B both accelerate the development of convection and amplifies the global reaction rate in the host solution. Both effects contribute to a larger dissolution flux and a faster storage of CO$_2$ into the host fluid. We compare our results with experimental results showing that reactions accelerate the development of buoyancy-driven fingering during the convective dissolution of CO$_2$ into aqueous reactive solutions of alkali hydroxides [5].


References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-D / 870

**Controlled depressurization of a hydrate-crusted gas capsule: insights from microfluidic experiments and phase-field modeling**

Xiaojing Fu$^{1}$; Joaquin Jimenez-Martinez$^{2}$; Luis Cueto-Felgueroso$^{3}$; Mark Porter$^{4}$; H. Viswanathan$^{4}$; J. Carey$^{5}$; Ruben Juanes$^{6}$

$^{1}$ Massachusetts Institute of Technology

$^{2}$ EAWAG-ETHZ

$^{3}$ Technical University of Madrid, Madrid, Spain
Understanding the evolution of a hydrate-crusted gas capsule during its depressurization is critical to elucidating the fate of methane bubbles escaping from seafloor seeps, a process that controls the impact of seafloor methane leakage on ocean biogeochemistry. While the physics of rising bubbles in a water column has been studied extensively, the process is poorly understood when a hydrate “crust” forms around the gas bubbles during their ascent. Understanding bubble rise, expansion and dissolution under these conditions is essential to determine the fate of bubble plumes of hydrate-forming gases such as methane and carbon dioxide from natural and man-made accidental releases.

In this work, we first present a high-pressure microfluidic experiment to study the controlled expansion of a hydrate-crusted bubble of Xenon in a water-filled and pressurized Hele-Shaw cell of 1 mm thickness. The system is initially pressurized from the Xenon gas inlet (i.e., from the Xe gas bubble) and maintained at a constant pressure of 7.5 MPa and constant temperature of 25°C for 18 hours to ensure equilibrium between Xenon-gas and liquid water. A layer of hydrate shell forms at the gas-liquid interface during this period. At the end of the 18 hours, the gas inlet is disconnected from the system, and the entire cell is depressurized from the surrounding liquid phase at a constant rate of 0.5 MPa/min. During depressurization, the expansion of the gas bubble is controlled by three processes: (1) the volumetric expansion of gas due to changes in pressure; (2) the rupture of the existing hydrate shell that encapsulates the expanding gas phase; and (3) the spontaneous formation of hydrate along the evolving gas-liquid interface. The interplay among these processes results in gas fingering leading to a complex labyrinth pattern, in contrast with the circular gas expansion that would occur in the absence of hydrate formation.

To reproduce the experimental observations, we propose a phase-field model that describes the formation and growth of a hydrate shell on an expanding gas-liquid interface. We design a Gibbs free energy functional for methane–water mixtures that recovers the isobaric temperature–composition phase diagram under thermodynamic equilibrium conditions. The proposed Gibbs free energy is then incorporated into the free energy of the three-phase system (gas-liquid-hydrate) to rigorously account for interfacial effects, phase separation and transformations dynamics: hydrate formation and disappearance, gas dissolution and exsolution. We introduce gas compressibility through a pressure-dependent density formulation. We model the hydrate phase as a highly viscous fluid phase with stress-yielding rheology to reproduce the rupturing behavior of the hydrate layer. We present high-resolution numerical simulations of the model, which illustrate the emergence of complex crustal fingering patterns as a result of gas expansion dynamics modulated by hydrate growth at the interface, as observed in the experiments.

References:

Click here to agree

Parallel 8-H / 581

Convergence Analysis of McMC Methods for Subsurface Flow Problems

Author(s): Arunasalam Rahunanathan

Co-author(s): Abdullah Mamun ; Felipe Pereira ; Samson Folarin

1 Department of Mathematics and Computer Science, Central State University
2 Department of Mathematical Sciences, University of Texas at Dallas
Corresponding Author(s): rahunanthana@gmail.com

In subsurface characterization using a history matching algorithm, we reconstruct the subsurface properties, such as distributions of permeability and porosity, with a set of limited data. As a history matching algorithm, Markov chain Monte Carlo (MCMC) method is effective for reconstructing permeability and porosity fields. The MCMC method is serial in nature due to its Markov property. Moreover, the calculation of the likelihood information in the MCMC is computationally expensive for subsurface flow problems. Running a long MCMC chain for a very long period makes the method less attractive for the characterization of subsurface. In contrast, several shorter MCMC chains can substantially reduce computation time and can make the framework more suitable to subsurface flows. However, the convergence of those MCMC chains should be carefully studied. In this talk, we consider multiple MCMC chains for a single-phase flow problem and analyze the chains for a reliable characterization.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-D / 909

Correlative microscopy approach to mix different scales in the porous dentin material

Elsa Vennat¹; Denis Aubry³

¹ CentraleSupelec

Corresponding Author(s): elsa.vennat@centralesupelec.fr

It is proposed in this talk to consider multiple resolution observations of dentine materials synthesized at multiple scales with a general inverse problem approach by combining confocal e.g. with SEM observations at different scales. Thus correlative microscopy aims to access a large range of scales for a given region by combining what is impossible by using one instrument alone.

Dentin is the bulk material of the tooth and presents a complex hierarchical structure. At the macroscopic scale, it can be seen as a first approximation as a homogeneous material located in between enamel and pulp cavity. But at the tissue level, it presents a microstructure made of tubules, peritubular dentin and intertubular dentin (entity dimension : a few microns). At a lower scale, the intertubular dentin is a composite made up of collagen fibers and hydroxyapatite crystals (entity dimension : 100nm).

Knowing the influence of the topology at each scale is of utmost importance for dental restoration. It is thus strongly needed to provide a robust and durable link between the restorative material and the same biomaterial. Local defaults will create stress concentration which will be the source of crack initiation either immediately or later due to cyclic loading and fatigue phenomena. On the other hand low resolution is often required to survey large regions, for example to locate and image sparse features such as critical features, but for which structural information is required at much higher resolution.

The proposed mathematical approach is viewed as an inverse problem: it starts a material structure at a given resolution with a given larger scale apparatus. Dispersed topography at diverse point sampled in the structure, find the fine fitted topography at the fine scale everywhere in the sample. To reach this goal we use concepts such as variational image restoration and texture synthesis together with PDE/FEM image analysis.

In this talk, dentin 3D imaging usingFocused Ion Beam-Scanning Electron Microscopy (FIB-SEM) and Confocal Laser Scanning Microscopy (CLSM) is performed and used in order to get some physical properties such as permeability and elasticity modulus at different scales.
Coulombic effects during conservative and reactive transport of charged solutes in homogeneous and heterogeneous porous media: Experiments and modeling

Muhammad Muniruzzaman; Massimo Rolle

1 Geological Survey of Finland
2 Department of Environmental Engineering, Technical University of Denmark

Corresponding Author(s): md.muniruzzaman@gtk.fi

Abstract

Transport of charged species in porous media is significantly affected by the electrochemical migration term resulting from charge-induced interactions among dissolved ions. Such electrostatic interactions during multicomponent ionic transport have been investigated both in diffusion-dominated systems [1-3] and, recently, in advection-dominated systems for steady-state plumes [4, 5]. In this work we study the electrochemical effects during transient conservative and reactive transport of ionic admixtures, under advection-dominated conditions, in homogeneous and heterogeneous domains by means of laboratory bench-scale experiments and numerical simulations. Experiments were performed in a quasi 2-D flow-through chamber under transient transport conditions by applying pulse injections of the electrolytes [6]. We performed extensive sampling (600 samples) and measurements of ions’ concentrations (1800 measurement points) at the outlet of the flow-through setup, at high spatial (5 mm) and temporal resolution (~0.017 pore volumes). Such sampling approach allowed us resolving the effects of charge interactions on the temporal breakthrough and spatial profiles of the cations and anions. The experimental results show remarkable differences, caused by the Coulombic effects, on the breakthrough curves and on mixing of the different ionic plumes. We evaluated the dilution behavior of individual charged species by experimentally calculating their flux-related dilution index as a metric of mixing.

Modeling of charged species and the interpretation of these experimental results require a Nernst-Planck based formulation with an accurate description of local hydrodynamic dispersion, as well as the explicit treatment of the cross-coupling between dispersive fluxes due to electrochemical migration. We used a recently developed 2-D reactive transport simulator [7], coupling the multicomponent ionic transport with the geochemical code PHREEQC by utilizing the iPhreeqc module, to quantitatively interpret the experimental results. The simulator allows us to reproduce the observed experimental outcomes and to directly quantify and visualize the electromigration effects by mapping the different components of ionic fluxes and their cross-coupling. Furthermore, we use this 2-D code to explore the impact of charge interactions in large-scale reactive transport scenarios with heterogeneous distribution of both physical and chemical properties.

Key words: electrochemical migration, multicomponent diffusion, breakthrough curves, iPhreeqc coupling, Coulombic interactions, dilution index, flow-through experiments

References:

(2007).

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-C / 230

Coupled chemo-mechanical fracture of silica in aqueous solutions

Louise Criscenti¹ ; Jessica Rimsza¹ ; Reese Jones¹ ; Edward Matteo¹

¹ Sandia National Laboratories

Corresponding Author(s): ljcrisc@sandia.gov

Crack propagation in silica may be enhanced in aqueous solution due to protonation of the silica surface and chemical reactions between the solution and strained siloxane bonds at the crack tip. To identify the coupled chemo-mechanical processes which govern silica fracture in the presence of pure and salt water, sub-critical fracture in amorphous silica has been investigated using molecular dynamics simulations and double-compression double-cleavage (DCDC) experiments. The molecular dynamics simulations have been performed with both a non-reactive and reactive force field. Using the reactive force field (REAXFF), slit cracks were introduced into models of amorphous silica and propagated as mode I fractures. The cracks were filled with reactive water molecules and different concentrations of NaCl. The simulation results confirm that the fracture toughness of silica in vacuum is greater than in aqueous solution. Using a reactive force field allows us to simulate water infiltration into the silica slit crack with reactivity: water dissociation allows for the hydroxylation of the silica surface, ion adsorption to the silica surface can affect the protonation of neighboring surface sites. The role of defect concentrations, crack tip radii, and solution composition on fracture toughness, surface structure, stress distributions, and crack depth will be discussed and qualitative comparisons between experimental and modeling results will be presented.


References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-E / 173

Coupled heat- and mass transport through a gas-filled nanopore in contact with a liquid

Author(s): Bjørn Hafskjold¹
Co-author(s): Laura Edvardsen ¹; Dick Bedeaux ²; Olav Galteland ²; Signe Kjelstrup ²

¹ Norwegian University of Science and Technology
² Norwegian University of Science and Technology, NTNU, Trondheim

Corresponding Author(s): bjorn.hafskjold@ntnu.no

Transport of water vapor through a membrane with nano- or micropores while being impermeable to liquid water is the basis for many fabrics and materials with widespread use. An application of the concept is membrane distillation (Lawson and Lloyd, 1997), where a temperature difference across the membrane drives transport of heat and mass. The transport is component selective and can purify the fluid. The transport processes through the membrane have recently been analyzed in terms of non-equilibrium thermodynamics (NET) (Kjelstrup and Bedeaux, 2008), resulting in a new understanding of the coupling between them and the roles of the thermodynamic driving forces.

In order to apply the NET formalism to specific cases, it must be supplied with data from experiments, theories, or computer simulations. The purpose of this paper is to examine some of the assumptions behind the NET formalism, such as the assumption of local equilibrium in the system, study the transport process mechanisms on the atomic scale, and provide case data for a model system by using non-equilibrium molecular dynamics (NEMD) simulations (Hoover and Hoover, 2015).

A cylindrical nanopore was filled with vapor in contact with a Lennard-Jones liquid. Equilibrium simulations were made to verify the model’s stability and generate equilibrium data against which non-equilibrium data could be compared. A temperature gradient was imposed and similar non-equilibrium data were generated. The data included surface tensions of flat and curved liquid/vapor interfaces as function of temperature, pressure differences across the surface, heat- and mass fluxes through the pore, and estimates of transport coefficients. System variables were temperature, temperature gradient, pore diameter, and vapor/pore wettability.

The main conclusion from this work was that the temperature gradient generated a pressure difference between the two bulk liquid regions shown in Figure 1. The vapor pressure in the pore, as well as the pressure difference, depended on the temperature and the temperature gradient. We found that the non-equilibrium data were consistent with the equilibrium data at the same local thermodynamic states, suggesting that the local equilibrium assumption is valid in this case.

References:

Click here to agree

Parallel 9-H / 413

Coupled thermal-hydraulic-mechanical simulation for enhanced geothermal system based on embedded discrete fracture model

Author(s): Tingyu Li¹

Co-author(s): Bo Yu ²; Dongliang Sun ²; Dongxu Han ²; Fusheng Yang ¹; Jinjia Wei ¹

¹ School of Chemical Engineering and Technology, Xi’an Jiaotong University, Xi’an 710049, China
² School of Mechanical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, China

Corresponding Author(s): 716668239@qq.com
Tingyu Lia, Dongxu Hanh, Bo Yub, Dongliang Sunh, Fusheng Yanga, Jinjia Weia
a School of Chemical Engineering and Technology, Xi’an Jiaotong University, Xi’an 710049, China
b School of Mechanical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, China
Corresponding authors: E-mail addresses: yubobox@vip.163.com (B.Yu).

As the most effective method for mining deep geothermal resources, the enhanced geothermal system
(EGS) has become a hot topic in the recent geothermal researches. To extract heat storage in the
Hot Dry Rock, hydraulic fracturing technology is used to form artificial flow aperture. Subsequ-
ently, the geothermal energy is extracted through heat carrying fluid cycle. The mining process
includes porous flow, heat exchange and deformation of rock, which is a typical thermal-hydraulic-
mechanical (THM) three field coupling problem. Recently, some scholars have carried out a prelimi-
inary numerical simulation study on the multi-field coupling in EGS [1-5]. However, there are still
two main shortcomings. First, the simulation of fractured rock mass is mostly based on continuum
hypothesis, which is only suitable for rock with relatively high porosity. This method shows large
error for EGS system dominated by several fractures. Second, the research on heat flow coupling
is not enough, which is the most basic and important aspect in EGS. Especially, the study of heat trans-
fer process and heat recovery efficiency under thermal-fluid coupling is not yet thorough. Therefore,
based on the embedded discrete fracture model (EDFM), the THM coupling model of the actual frac-
tured rock mass is established. Two energy equations are used to describe the heat transfer process
in the matrix and fracture respectively. Finite volume method (FVM) is applied to discrete energy
equation, two point flux approximation (TPFA) method for porous flow equation and finite element
method (FEM) for solid skeleton deformation equation.

All variables are solved simultaneously through the Newton-Raphson iterative method, the calcu-
lation of the Jacobian matrix uses automatic differentiation algorithm. The influence of reservoir
heterogeneity, anisotropy, injection rate, injection pressure and well spacing on the exploitation
temperature of EGS system is emphatically analyzed.

References:
[1] Cao W, Huang W, Jiang F. A novel thermal–hydraulic–mechanical model for the enhanced geother-
[3] Xu C, Dowd P A, Tian Z F. A simplified coupled hydro-thermal model for enhanced geothermal
[4] Ghassemi A, Zhou X. A three-dimensional thermo-poroelastic model for fracture response to injec-

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-C / 441

Coupling of different numerical approaches for efficient simula-
tions in porous and fractured media

Stefano Berrone¹ ; Andrea Boriso² ; Sandra Pieraccini² ; Stefano Scialò²

¹ Politecnico di Torino, Italy
² Politecnico di Torino

Corresponding Author(s): stefano.scialo@polito.it

The simulation of flows in poro-fractured heterogeneous media is a challenging task, manly as a
consequence of the geometrical complexity of the domain. Fractures in the porous matrix are di-
mensionally reduced to co-dimensional interfaces, in order to avoid the resolution of the scale of
the fracture thickness, which can be orders of magnitude smaller than the typical dimensions of
the computational domain. Fractures, then, act as irregularity interfaces for the solution, and stan-
ard numerical approaches based on finite elements or finite volumes are required to conform to
these interfaces in order to capture the correct behavior. New numerical approaches are proposed
here, born from the coupling of standard discretization techniques with recent and non-conventional methods, such as the Virtual Element Method (VEM), [1,2] or the optimization based non-conforming Finite Elements [3 4 5]. This new family of techniques overcomes the need of conformity at the interfaces. Further, the computational domain can be easily split in sub-domains and the most convenient discretization approach can be used in different regions of the domain, thus effectively tackling geometrical complexity and heterogeneity.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 738

Custom-built wetting properties in microchips with geomaterials by using layer-by-layer (LbL) assembly technology

Bin Pan¹ ; Yaqi Zhang¹ ; S. H. Hejazi² ; Amir Sanati-Nezhad³

¹ a. Subsurface Fluidics and Porous Media Laboratory, Chemical and Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada. b. BioMEMS and Bioinspired Microfluidic Laboratory, Department of Mechanical and Manufacturing Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada.

² Subsurface Fluidics and Porous Media Laboratory, Chemical and Petroleum Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada.

³ a. BioMEMS and Bioinspired Microfluidic Laboratory, Department of Mechanical and Manufacturing Engineering, University of Calgary, Calgary, AB T2N 1N4, Canada. b. Centre for Bioengineering Research and Education, University of Calgary, Calgary, AB T2N 1N4, Canada

Corresponding Author(s): bin.pan1@ucalgary.ca

Wettability is known to have an enormous impact on oil recovery in the petroleum industry and efforts are being made to assess the role of such conditions. This work creatively tailors the microchip surface wetting property by using rock-forming mineral coatings. The mineral surfaces are created in microchips by using the novel layer-by-layer (LbL) assembly technology. The formed mineral surfaces are equipped with varying roughness and wetting properties when different types of rock-forming minerals. The relationship between surface wettability and roughness is quantitatively studied. The fluid dynamics in the confined geometries with varying surface properties including wettability and roughness is analyzed. As an example of applying the developed microchip devices with custom surfaces to solve practical subsurface questions, the wettability alteration during the chemical enhanced oil recovery (EOR) processes, like surfactants, foam and nanoparticles, are studied. This work aims to study the physics of solid-liquid interaction (wetting property) in subsurface porous media by microfluidics technology and thus facilitate the research of chemical EOR measures in the petroleum industry.

References:
DEM-CFD coupling for the simulation of filter cake formed due to poly-dispersed particles.

Author(s): Ruturaj Deshpande
Co-author(s): Oleg Illiev; Sergiy Antonyuk

*Fraunhofer ITWM
*Fraunhofer ITWM, Kaiserslautern, Germany
*TU Kaiserslautern

Corresponding Author(s): oleg.illiev@itwm.fraunhofer.de

In this study, we analyze the filter cake formed due to mono and bi-dispersed spherical particles. The particle-particle, particle-filter interactions are simulated using Discrete Element Method (DEM) and the fluid flow is simulated using Finite Volume Method (FVM). The computation of the two-way particle-fluid interaction is the challenging part in the numerical studies mainly due to the calculation of the drag force. The fluid drag force in this study is calculated by using the poly-dispersed drag model suggested by Beetstra (2005). The numerically predicted void fraction of the filter cake formed due to the mono and the bi-dispersed particles is compared with the sedimentation experiments in the literature. We then analyze the effect of factors affecting the filter cake formation i.e. the particle-particle interaction parameters (the coefficients of the sliding and the rolling friction, the surface energy) and the poly-dispersity (the particle mass fraction ratio). We observed that, in general with the increase of the coefficient of sliding and rolling the predicted void fraction increases. Further neglecting the attractive forces between the particles under predicts the void fraction. At sufficiently higher particle Reynolds number the filter cake formed due to the mono and the bi-dispersed particles undergoes consolidation. At a constant Reynolds number pressure drop across a filter cake formed due to bi-dispersed particles increase with the increase in the mass fraction of the bigger particles.

References:

Parallel 10-E / 902

DEVICE FOR PROCESS CHARACTERIZATION OF CERAMIC MATRIX COMPOSITES FABRICATED BY LIQUID INJECTION

Alessandro Scola; Edu Ruiz; Nicolas Eberling-Fux; Sylvain Turenne

*Polytechnique Montreal
*SAFRAN Ceramics
Corresponding Author(s): a.scola@polyml.ca

Nowadays, ceramic materials are used in many industries. Ceramic materials are well known by their high strength and excellent thermal and chemical stability. In addition, most of ceramics retain acceptable mechanical properties at temperatures higher than 1000 °C. However, the low impact toughness of these materials limits their use in industries such as aerospace. The porous nature of the material allows cracks to propagate with low energy thus making the material susceptible to brittle fracture. Ceramic Matrix Composites (CMC) have been developed to combine the advantages of bulk ceramics, their low density and their excellent mechanical properties at elevated temperatures, with the advantages of fiber reinforced composites offering better tolerance to damage. Thus, making possible the use of CMC in environments requiring some high mechanical properties at elevated temperatures and at a high level of confidence.

An approach to create such a material is to generate a Weak Matrix Composite (WMC). This method proposes to control the residual porosity of the matrix to improve the impact properties. WMC is particularly applicable to Oxide/Oxide CMC since conventional manufacturing methods inevitably leave a high matrix porosity distribution (in the order of 20 to 30% of the total volume ratio). However, obtaining a matrix microstructure with fine and evenly distributed pores remains hard to achieve with the actual fabrication processes typically used in the industry. This is due to the heterogeneous nature of the ceramic particles used in liquid molding of CMC.

In this work, a novel slurry impregnation and filtration method was developed to fabricate Oxide/Oxide CMC. This method consists of a transverse impregnation of the fibrous reinforcement, which results in a quicker filtration than typical in-plan impregnation. Due to the though-thickness filtration and compaction, this process results in composites with higher density and lower residual porosities than traditional processes.

In this study, an instrumented device has been developed to characterize the through-thickness impregnation of ceramic fibers by a slurry filled with ceramic particles. The device, based on the principle of Darcy’s column, integrates flow measurements, pressure and displacement control and filtration measurements. This instrument was first used in the present work to characterize the permeability of the fibrous reinforcement and filtration media. It was then used to study the formation of the ceramic cake by filtration of the ceramic particles. Slurries containing different concentrations of alumina particles were filtered under different pressure conditions to optimize the cake formation and filling of fibrous reinforcements with the lowest porosity. Furthermore, a mathematical model based on Darcy’s law was developed in this study to predict the rate of filtering and cake formation during injection using the permeability and filtration data measured with the experimental device. This mathematical model allows to predict the filtration time needed to produce a densified CMC with good accuracy.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 276

DLVO Interaction Energies between Hollow Spherical Particles and Collector Surfaces

Chongyang Shen¹; Scott Bradford²; Zhan Wang³; Yuanfang Huang⁴; Yulong Zhang⁴; Baoguo Li¹

¹ China Agricultural University
² USDA ARS
³ Shenyang Agricultural University
⁴ yfhuang@cau.edu.cn

Corresponding Author(s): chongyang.shen@cau.edu.cn
The surface element integration technique was used to systematically study Derjaguin-Landau-Verwey-Overbeek (DLVO) interaction energies/forces between hollow spherical particles (HPS) and a planar surface or two intercepting half planes under different ionic strength conditions. The inner and outer spheres of HPs were concentric (CHP) or in point contact (PHP). In comparison to a solid particle, the attractive van der Waals interaction was reduced with increasing inner radius of the CHP, but the reduction effect was less significant for the CHP at smaller separation distance. Increasing the inner radius for CHP therefore reduced the depths of the secondary minima, but had minor influence on the energy barrier heights and depths of the primary minima. Consequently, increasing inner radius reduced the potential for CHP retention in secondary minima, whereas did not influence the retention in primary minima. For PHP these interaction energy parameters and colloid retention depended on the orientation of the inner sphere relative to interacting surface. In particular, the van der Waals attraction was significantly reduced at all separation distances when the inner sphere was closest to the interacting surface, and this diminished retention in both secondary and primary minima. The PHP retention was similar to that of CHP when the inner sphere was farthest from the interaction surface. These orientation dependent interaction energies/forces resulted in directional bonds between PHPs and the formation of aggregates with contact points of the primary PHPs facing outward. The findings in this study have important implications for the design and utilization of HPs in soil remediation and colloid assembly.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-H / 154

Decoupled, energy stable scheme for Cahn-Hilliard phase field model of two-phase incompressible flows

Guangpu Zhu¹; Shuyu Sun²; Jun Yao¹

¹ Research Center of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum (East China)
² Computational Transport Phenomena Laboratory, Division of Physical Science and Engineering, King Abdullah University of Science and Technology

Corresponding Author(s): b16020069@s.upc.edu.cn

In this paper, an efficient, totally decoupled and energy stable scheme is presented for the Cahn-Hilliard phase field model of two-phase incompressible flows. The rigorous proof of unconditional energy stability for the semi-implicit scheme and the fully discrete scheme are provided. The scalar auxiliary variable (SAV) approach is implemented to solve the Cahn-Hilliard equation while a splitting method based on the pressure stabilization is used to solve the Navier-Stokes equation. At each step, the scheme involves solving only a sequence of linear elliptic equations, including a pressure Poisson equation. An efficient finite difference spatial discretization on the staggered grids is applied to verify the accuracy and efficiency of the proposed schemes. Numerical results in both 2D and 3D demonstrate that the proposed schemes are very efficient, accurate and energy stable.

References:

Click here to agree

Parallel 5-B / 814

Deforming unsaturated media: a unified approach
Jacques Huyghe\textsuperscript{1} ; Ehsan Nikooee\textsuperscript{2} ; S.M. Hassanizadeh\textsuperscript{3}

\textsuperscript{1} University of Limerick  \\
\textsuperscript{2} Shiraz University  \\
\textsuperscript{3} Utrecht University

Corresponding Author(s): jacques.huyghe@ul.ie

The finite deformation of an unsaturated porous medium is the result of a complex interplay between capillary effects, interfacial area propagation, pressure diffusion and large deformations of the solid skeleton. Discrete approaches provide a means to integrate the physics of capillarity with deformation. However, discrete approaches only open the road to simple cases. The authors analysed the interplay of deformation and capillarity in a continuum thermodynamic analysis \cite{Huyghe2018}. An expression for Bishop’s effective stress directly links to the deformation dependent Brooks and Corey’s water retention curve by the restrictions on the constitutive relationships of an unsaturated medium. The resulting expression for the effective stress parameter is reasonably consistent with experimental data from the literature. In the present presentation, the authors will attempt to include interfacial area as an independent variable to create a model that predicts the hysteresis observed in drainage-imbibition and in stress-strain relationships.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-H / 735

Delaying Steam Breakthrough in a Fractured Heavy Oil Reservoir - Strategies and Outcomes

German Abzaletdinov\textsuperscript{1} ; Ipsita Gupta\textsuperscript{2} ; Sergey Durkin\textsuperscript{3}

\textsuperscript{1} Research Assistant  \\
\textsuperscript{2} Louisiana State University  \\
\textsuperscript{3} Ukhta State Technical University

Corresponding Author(s): gabzal@lsu.edu

It is well known that naturally fractured reservoirs very often represent the behavior of dual porosity systems, however, it is also similarly known that simulating flow and transport of oil and gas through dual porosity systems is computationally expensive, especially if simulating enhanced oil recovery (EOR) processes. Most of the simulation work that is thus done for full field and/or sector models use the single porosity approach for computational efficiency. In this study, the objective is to test both single as well as dual porosity models at the full-field scale for history matching and development strategies of a naturally fractured heavy oil reservoir in Russia. Because of computational expenses, high performance computing (super computers) is employed to assess the extent of modelling capabilities that can be replicated today with currently existing computational technologies for thermal EOR processes like SAGD and thermogel injection amongst others.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-D / 1068
Deliquescence behavior of salts confined in small pores

Tanya Talreja-Muthreja\textsuperscript{None} ; Kirsten Linnow\textsuperscript{None} ; Michael Steiger\textsuperscript{None}

**Corresponding Author(s):** tanya.talreja@chemie.uni-hamburg.de

The relative humidity at which a salt absorbs water vapor from the atmosphere spontaneously to form a saturated solution is called the deliquescence relative humidity (DRH) of the salt. In comparison to the DRH of bulk salt crystals, the DRH of levitated salt nanocrystals increases with decreasing crystal size\textsuperscript{[1,2]}. Even in case of salts confined in pores smaller than 100 nm the DRH is no more equivalent to that of bulk crystals. It is strongly affected by the curvature of the liquid-vapor interface, when the pore size of the porous material gets smaller than 100 nm. To our knowledge, experimental investigations about the influence of confinement below 100 nm in diameter on the deliquescence humidity of a salt are not yet carried out.

The experimental work focuses on the water uptake behavior of different salt-silica-composites with pores smaller than 100 nm carried out to investigate the deliquescence behavior of confined salt. Porous materials like mesoporous SBA-15 and controlled porous glasses are impregnated with NaCl and KNO$_3$-solutions preventing over-filling of the available pore volumes. The experimental results of the water sorption measurements of bulk salts, pure host materials and the composites reveal a significant decrease of the deliquescence humidity (DRH) of the salt with decreasing pore size. A thermodynamic model approach, based on combined use of the Young-Laplace equation, the Kelvin equation and the Pitzer ion-interaction model, is used to predict the sorption behavior of salts confined in the respective pore sizes. The calculations match well with the experimental results that the main reason for the decrease of the relative vapor pressure over the salt solution in the unsaturated pore is the concave curvature of the liquid-vapor interface. Similarly, this model approach show, that the increase in DRH of levitated nano-sized salt crystals\textsuperscript{[1,2]} is due to the convex curvature of the liquid-vapor interface, whereas the effect of increase in solubility with decreasing crystal size is low. Further experimental work focuses on the water uptake behavior of porous materials containing salts, which form higher hydrated phases before they deliquesce.

**References:**


**Acceptance of Terms and Conditions:**

Click here to agree

**Parallel 5-F / 183**

Design Pattern Enabling the Flexible Integration of Effects into a Basis Flow Model

Tatiana Reiche\textsuperscript{None}

**Corresponding Author(s):** tatiana.reiche@grs.de

The assessment of the long-term safety of a deep underground repository for radioactive waste requires a comprehensive understanding of the system and appropriate numerical tools. RepoTREND is a final repository simulator being developed by GRS for simulating

- the release of contaminants and
- their transport through the near-field and far-field to the biosphere, including
- the estimation of the radiological consequences for man and environment.

It will be applicable to different concepts of final repositories in different host formations.

In a typical repository simulation the model area is extremely heterogeneous. Neighbouring grid elements can essentially differ with respect to their properties and the relevance of the effects that
have to be considered additionally to the underlying basic processes, such as the two-phase flow in porous media. Such heterogeneities can lead to the necessity to vary the basic equations over the model regions. For instance, the rock convergence dynamically changes the pore volume in some region. The convergence process is controlled by a number of additional factors, and the change of the pore volume is described by a nonlinear differential equation that has to be integrated into the global equation system for the relevant region. The relevance of effects depends on the environment parameters and may change during the simulation time. For example, rock convergence gets irrelevant as soon as a final value of porosity is reached.

During a simulation of the processes in a repository for radioactive waste, numerous different effects have to be considered. Specific challenges in developing the structure of a simulator program are to enable a flexible choice of effects for different regions of the modeled area, their combination during a simulation and an easy way to extend the program by new effects.

The paper presents a concept for realizing these requirements by flexible introduction of effects into the simulation. The concept consists of the following steps:

- Define a family of Effects. An Effect class encapsulates the related parameters and effect-specific routines for pre-/post processing for a time/iteration step.
- Define a family of Expert objects that capture a current system state (relevant effects, basic model) and encapsulates the interaction of relevant Effects. These Expert objects have to be dynamically selectable corresponding to the current system state in the relevant regions. Expert objects enable the loose coupling of data structure. By using Expert objects the explicit dependency between Effect objects can be avoided. This concept enables the interaction of objects to be varied and modified independently of the objects themselves.

This concept ensures the implementation of new effects in an easy way according to the predefined pattern, flexibility, transparency and reusability in extending and developing the program.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-E / 857

**Design of Pneumatic Fracturing Experiments for Rare Earth Elements Recovery by Support of X-ray Micro Computed Tomography Imaging**

Author(s): Gerhard Zacher¹
Co-author(s): Matthias Halisch ; Wilfried Hüls

¹ GE Sensing & Inspection

Corresponding Author(s): gerhard.zacher@bhge.com

**Introduction**

The Development of an environmentally sustainable method for the extraction and processing of Rare Earth Elements (REE) is an ongoing study as the state of the art exploration like e.g. in China leads to a significant impact to the environment in terms of water pollution, destruction of the biosphere and erosion. For a mining project in Madagascar it is therefore planned to induce fractures and fissures in the subsurface deposit by pneumatic fracturing for improvement of permeability to be able to extract REE by controlled leaching (European Commission, 2014, SGS, 2016). To perform lab experiments clay samples were collected on site. For preconditioned humidity and pressure
values inside a triaxial test device (see figure 1) tailored pneumatic pulses were injected by using compressed inert gas.

Figure 1 Triaxial test device

Experimental Setup

The equipment used is a modified large triaxial cell for soil sample diameter of 7 cm and height of 14 cm. Its modification was mainly on the bottom base wherein a hole was made through the center to facilitate access to the bottom of the specimen while under an applied confining stress. A needle of 3.8 cm length was used to create an injection well inside of the sample. The loading conditions shall simulate an overburden pressure for deposit depth (d) between 5 m and 20 m. The focus of these tests was to investigate fracture-initiation pressure as well as fracture growth. Parameter variations are pulse loading height, time period and number of individual pulses. Depending on the loading, different fractures for anisotropic and isotropic conditions have been observed.

Results

Due to X-ray micro-computed tomography (µ-CT) the structure of fractures and fissures inside of the sample have been very well monitored according to each experimental loading step. For test series 1 (see figure 2) the resulting fractures are located close to the top of the injection well as shown in the 3 orthogonal slice views. The 4th view gives a zoomed 3D visualization of the segmented fracture system.

Figure 2 This X-ray CT result indicates smaller cracks with punctual origin (d = 17.5 m).

For another test series (no. 3) the pulse loading height was 3 times higher which led to a continuous fracture through the whole sample width along the injection well (see figure 3).

Figure 3 Another CT result shows a disruptive fracture in all 4 views (d = 10 m).

Conclusions and Outlook

Therefore, as a result of our research, we are confident that starting with deposit conditioning by pneumatic fracturing it is possible to apply a leaching mining and processing procedure, which is environmental friendly, more efficient and faster than those methods applied traditionally.

References

[1] European Commission, 2014: Communication from the commission to the European Parliament, the Council, The European Economic and Social Committee and the committee of the regions on the review of the list of critical raw materials for the EU and the implementation of the raw materials initiative, [eur-lex.europa.eu/legal-content], pp. 7.


References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-F / 939

Detailed numerical simulation of capillary pressure curve hysteresis
Ashraful Islam ¹; Bernd Crouse²; Ganapathi Balasubramanian ¹; David M. Freed ¹

¹ Exa
² Exa Corporation

Corresponding Author(s): bernd.crouse@3ds.com

We present a detailed analysis of a “full physics” simulated drainage-imbibition capillary pressure hysteresis on a packed sphere test case, with particular focus on the fluid displacement mechanisms. The chosen LBM-based flow simulator includes a surface-element boundary scheme to ensure accurate surface treatment and robust handling of arbitrary geometries even in low grid resolution scenarios. This simulator also allows specification of the wetting condition, which is essential for multi-phase flow.

During primary drainage, oil (non-wetting fluid) is pushed into a strongly water-wet porous media displacing water. The oil pressure is slowly increased and resulting water saturation values are measured. The entry pressure of the simulated drainage capillary pressure curve is compared to a theoretically derived reference solution based on the Young-Laplace law and geometric considerations. It is shown that the entry pressure is consistent with the inscribed radius of the critical pore throat, and it is further demonstrated that the entire drainage capillary pressure curve depends primarily on the geometry of the porous medium.

The final state of the primary drainage simulation is used as the initial condition of the main imbibition simulation. The oil pressure is slowly reduced to allow water to imbibe the pore space. By plotting the resulting primary drainage and main imbibition capillary pressure curves together, it is seen that for a given water saturation value, the pressure at which water displaces oil (imbibition) is different compared to the pressure at which oil displaced water (drainage), demonstrating capillary hysteresis.

Detailed analysis reveals that the imbibition curve depends strongly on both the curvature of the fluid-fluid interface and the solid geometry. Therefore, accurate prediction of capillary pressure curve hysteresis requires direct simulation of both fluid phases and correctly capturing the detailed interface topology at each pressure condition. This in turn implies that geometry and surface wetting condition are important – geometry simplification and unrealistic contact angle distribution will likely lead to significant inaccuracies.

Another aspect of the presented analysis is the displacement time-scale. During the drainage process, as pressure is slowly ramped up, the change of water saturation is small until the entry pressure has been overcome. Oil then quickly streams into the now accessible pore space. This phenomenon, known as a Haines jump, can also be observed during the imbibition process.

Finally, the simulation method is used to predict the drainage-imbibition capillary pressure cycle on a real sandstone rock sample. It is shown that the same basic mechanisms observed for packed spheres are also present for complex pore spaces.

References:

Xiaowen Shan, Hudong Chen, "Lattice Boltzmann model for simulating flows with multiple phases and components, Physical Review E, 1993


Gary R. Jerald, Joanne Fredrich, Nathan Lane, Qiang Sheng, Bernd Crouse, David M. Freed, Andrew Fager, Rui Xu, "Validation of a Workflow for Digitally Measuring Relative Permeability", SPE-188688-MS, 2017

Click here to agree

Poster 4 / 1013

Determination and Prediction of VOC Adsorption Performance Data of Activated Carbon Based Filter Media for Indoor Air Purification

Author(s): Roman Ligotski ¹
Co-author(s): Uta Sager 2; Christof Asbach 2; Frank Schmidt 1

1 University of Duisburg-Essen
2 Institute of Energy and Environmental Technology

Corresponding Author(s): roman.ligotski@uni-due.de

Determination and Prediction of VOC Adsorption Performance Data of Activated Carbon Based Filter Media for Indoor Air Purification

Roman Ligotski (1), Uta Sager (2), Christof Asbach (2), Frank Schmidt (1)
1 Nanoparticle Process Technology, Department of Mechanical and Process Engineering, University of Duisburg-Essen, Lotharstraße 1, D-47057 Duisburg, Germany
2 Institute of Energy and Environmental Technology, Bliersheimer Str. 60, D-47229 Duisburg, Germany
email for correspondence: roman.ligotski@uni-due.de

Over the last few years the adsorptive purification of the gas phase in HVAC-systems has got more and more focussed. One of the reasons for this trend is the fact that people in Europe and North America spend 85-90 % of the day time in indoor environments, i.e. vehicle cabins and especially buildings. During this time they can be exposed to a variety of harmful gaseous compounds. Regarding adverse health effects VOCs (volatile organic compounds), which can be released from different indoor sources such as building materials, cleaning agents and cosmetics, are an important group of specific indoor contaminants. In addition, due to energy saving HVAC-concepts, parts of the air in buildings get recycled and mixed with preferably small amounts of fresh air before being re-introduced into the building. This could lead to an accumulation of VOCs in the indoor air. The latter can be avoided by an efficient adsorptive removal of these compounds in ventilation systems. For the validation of adsorptive indoor filter media the relatively new international standard DIN EN ISO 10121-1 recommends toluene as a model compound for VOCs as challenge vapor with a concentration of 9 or 90 ppm in conditioned air (T=23±0.5 °C, RH: 50±3 %). The filter media tests according to ASHRAE 145.1 are carried out at a toluene concentration of 100 ppm. However, VOC concentrations in real buildings are typically one or more orders of magnitude lower than in the standard tests. Carrying out tests at more realistic concentrations would require a much longer period of time (weeks or months). However, the knowledge of the behavior of adsorptive filters under indoor relevant conditions is useful to compare the quality of filters and to approximate their service time. To face this problem the Wheeler-Jonas [2] and Yoon-Nelson [3] equation were used to predict the adsorption performance data at low concentrations down to 0.1 ppm using test results from standard tests at higher concentrations. The possibilities and limits of the predicting methods will be presented for the exemplary system of toluene and activated carbon (AC) based filter media with different properties in comparison with experimental data.

Besides the concentration, the considered standards recommend RH values which can differ from the humidity of indoor air. Higher humidity content can result in a reduction of adsorption capacity and slower adsorption kinetics of toluene. Hence the effect of higher relative humidity (up to 90 % RH at 23 °C) on the adsorption performance of toluene on filter media with various characteristics of the AC (pore size distribution and surface chemistry) was also part of the study. The results will be discussed in the presentation.

References:

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 7-B / 169

Determination of solid-phase conduction shape factor for spherical-void-phase REVs generated by a random discrete element model

Jeremy Vu¹ ; Anthony Straatman¹

¹ Western University

Corresponding Author(s): astraatman@eng.uwo.ca

This article describes the direct comparison between pore-level computations on a spherical-void-phase (SVP) porous material and volume-averaged computations done for the same domain. Pore-level simulations are conducted on random SVP geometries generated using the Discrete Element Modelling (DEM) approach developed by Dyck & Straatman [1] over a range of flow and heating conditions. Pore-level simulations for cases of constant wall temperature require nearly 17,000,000 tetrahedral elements and provide data that are used to establish the fluid permeability and interstitial convection coefficient of the REVs under consideration. Additional pore-level simulations are then conducted on the same REVs except treating it as being heated on one side by a constant-temperature substrate. These simulations require discretization of both the fluid and solid phases of the REV and require nearly 32,000,000 tetrahedral elements to produce grid-independent solutions of forced convection heat transfer. Analogous conjugate heat transfer simulations are done using a volume-averaged solver on the same domain using the closure parameters established in the pore-level simulations. These simulations require only 5800 hexahedral elements to achieve grid convergence to better than 1%. Comparison of the conjugate results from the pore-level and volume-averaged solvers provides data to establish a solid-phase conduction shape factor that is necessary to modify the diffusion term in the volume-averaged solid-phase energy equation. The solid-phase conduction shape factor is dependent only on the geometric structure of the porous domain and accounts for the additional resistances in the conduction path due to elongation and area changes along the path [2-5]. Even though there is no analytical means for establishing the conduction shape factor for complex geometric models, it is shown that the factor can be established for a particular geometric model on the basis of comparisons for a single heating condition. Subsequent simulations comparing the pore-level and volume-averaged results show that the accuracy of volume-averaged computations is enhanced by as much as 20% with the proper characterization of the solid-phase conduction shape factor.

References:

Click here to agree

Parallel 2-H / 351

Determining the Impact of Mineral Composition and Roughness in Multiphase Flow through Fractures

Author(s): Javier E. Santos¹
Co-author(s): Maša Prodanović ² ; Christopher J. Landry ³
Fractures are ubiquitous in the subsurface, and provide primary pathways for fluids traveling underground. The roughness and wettability of the fractures in the subsurface cause a major impact on multiphase flow behavior. Nevertheless, published analytical solutions for multiphase flow properties of fractures fail to account for the complexity of the surface mineralogy heterogeneity and its effect on production from fractured reservoirs. Since analytical solutions for fracture surfaces with heterogeneous wetting properties are very limited, we propose a direct simulation approach. The purpose of this work is to correlate the reduction of relative permeability in multiphase flow through fractures with different mineralogy and surface roughness.

Utilizing the Shan-Chen multiphase model of the lattice-Boltzmann method (LBM) we are able to simulate oil and water displacement in 3D fractures. Simulation domains were extracted from 3D micro-CT scans and digitally synthesized. A surface interaction parameter is adjusted to mimic the time-dependent microscale wettability of the different minerals present in fractures. We then map the mineralogy of surfaces obtained by SEM imaging and integrate them with contact angle measurements on individual minerals to provide input for the simulations. We also account for the possible change in contact angle over time due to wettability alteration. These simulations were carried out at the Texas Advanced Computing Center.

In this work, we quantify the effect of different mineralogy arrangements and wetting states on the relative permeability. From these measurements, we derive correlations based on fracture aperture, surface roughness, and the spatial distribution of minerals.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 2 / 426

Development of Embedded Discrete Multi-Fractures Model for Simulation of Fractured Reservoirs

Renjie SHAO³ ; Yuan DI¹ ; Dongli ZHANG² ; Yanyan ZHAO²

¹ Peking University
² Exploration & Production Research Institute, SINOPEC
³ University of Texas at Austin

Corresponding Author(s): shaorenjie@pku.edu.cn

Accurate and efficient numerical simulation of fractured reservoirs is important and challenging. Conventional dual porosity and dual permeability(DP/DK) models are efficient but not accurate, especially when fracture-diagnostic tools make it easier to get the detail of the complex fracture networks. Discrete-fracture models(DFM) have been developed to use information of fracture networks, which is still limited for its computational inefficiency. Recently, Embedded Discrete Fracture Model (EDFM) became a promising study orientation to overcome such problems.

In this study, we improve the EDFM approach by embedding discrete multi-fractures instead of simple fracture pieces in the matrix domain. Multi-fractures here stand for parts divided from fracture network, each consisting of multiple fractures and their intersection. This model has a comparative advantage: the embedded fracture network can be divided into larger and more complex parts with arbitrary shapes and sizes when meshing grid. And each complex part can be considered as a whole. The calculation of conductivity between NNCs (Non-neighboring Connections) is the core of EDFM. We expound that the key to calculate conductivity of NNC is to approximate a local pressure field. Thus a new calculation method based on a more reasonable local pressure distribution has been developed. This method is suitable for the multi-fractures model and more accurate than the one used in original EDFM especially when matrix grid is coarser.
We demonstrate the accuracy and efficiency of the new conductivity calculation method and the embedded discrete multi-fractures model by performing a series of case studies with CarstSim simulator and comparing the results with the original EDFM and fine-grid models. We also present two numerical case studies to demonstrate the applicability of our method in naturally fractured reservoirs.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-E / 465

**Deviations from Darcy’s law studied by non-equilibrium molecular dynamics simulations**

Olav Galteland¹; Bjørn Hafskjold¹; Signe Kjelstrup¹; Dick Bedeaux¹

¹ Norwegian University of Science and Technology

Corresponding Author(s): olav.galteland@ntnu.no

It has been known for a long time that there are cases where Darcy’s law does not apply, also for single phase flow with small capillary numbers [1–4]. The flow rate has for some cases been found to be proportional to the pressure gradient raised to the power 1/n where n = 1. For other cases it has been found to be a threshold pressure, below which no flow occurs.

Non-equilibrium molecular dynamics simulation is an excellent tool to study flow in porous media. We have used a modified Lennard-Jones/Spline potential which makes it possible to model a wide range of systems with varying pore sizes, interface tensions and fluid viscosity. The Reflective Particle Method has been used to create a pressure difference across the porous medium [5]. The red particles are fluid and the blue particles are pore particles with a fixed position.

We present results for single and two-phase flow varying the context of wetting fluid, porosity, average pore diameter, and interface tensions. The results are interpreted using non-equilibrium thermodynamics for porous materials, a new theory. On this bases we propose various reasons for deviations from Darcy’s law.

Acknowledgement

The calculation power is granted by The Norwegian Metacenter of Computational Science (NOTUR). Thanks to the Research Council of Norway through its Centres of Excellence funding scheme, project number 262644, PoreLab.

References:

Poster 4 / 1102

Diagenetic Mechanism of Porous Carbonate Reservoir and Its impact on Reservoir

Fengfeng Li¹ ; Yichang Yu¹ ; Rui Guo¹

¹ Research Institute of Petroleum Exploration and Development

Corresponding Author(s): 1522188426@qq.com

The Mishrif Formation in the Hafaya Oilfield is mainly characterized by porous carbonate reservoir with large marine biology, different sediments and complex diagenesis. Reservoir in this area has diverse pore types, poor correlation between porosity and permeability, poor well logging response and reservoir evaluation is difficult. The diagenetic patterns of different microfacies have been established based on core, cast thin film, mercury intrusion data and scanning electron microscopy, and the diagenesis mechanism of porous carbonate rocks and the reformation of reservoirs have been clarified. Microfacies in the Mishrif Formation control the types of biomask particles, and the biological shells have different ability in resistance dissolution. Selective dissolution leads to various moldic pore. The environment determines the type of diagenesis. In briny environment, the main types are mud crystallization, biogenicagency and rim cementation. The nemorphism and selective dissolution are the main types of diagenesis in freshwater environment. Hypergene zone is dominated by weather erosion and non-selective dissolution, In burial environment, the main diagenesis are coarse-grained cemented and dolomitization. The type of diagenesis determines the tendency of reservoir reformation, in which the compaction, the pressolution and the cementation reduce the porosity and the dissolution increases the porosity and provides the cementing material. The dolomitization has two sides, if the calcite is replaced, porosity increases and if the pore is filled, porosity decreases. The diagenetic stage controls the pros and cons of reservoir reformation. The early cementation and late dissolution is favorable for pores protection. The late dissolution and early cementation is the most unfavorable. The results show that reservoir reformation is the comprehensive superimposition of sedimentary materials, diagenetic stages, environments and types. Sedimentation provides the material and environment determines the diagenesis type and sequence. The type and period of diagenesis determine the reformation tendency of reservoir in the Mishrif Formation. It is of great significance to clarify the mechanism of diagenesis for the reservoir evaluation and the potential analysis of reserves.

References:

Poster 4 / 1097

Differential diagenesis and pore evolution mechanism of restricted platform carbonate reservoirs

Yichang Yu¹ ; Xinmin Song¹ ; Rui Guo¹ ; Hangyu Liu¹ ; Fengfeng Li¹

¹ Petrochima Research Institute of Petroleum Exploration and Development
Corresponding Author(s): yuyichang2013@163.com

The reservoir heterogeneity of the restricted platform in the Mishrif formation of Iraq HF oil field is strong, different microfacies experience different diagenesis and pore evolution process, and the seepage characteristics are different. Therefore, to clarify the differential diagenesis and pore evolution mechanism is the basis of improving development effect. Based on core observation, physical property, mercury injection capillary pressure test, casting thin sections, scanning electron microscopy, cathodoluminescence, electron probe and fluid inclusion analysis, the sedimentary characteristics, diagenesis and the evolution process of pore are systematically studied. The results show that: (1) The restricted platform can be divided into bioclastic shoal, inter-shoal and intraplatform shallow. The bioclastic shoal is located in high landform of strong hydrodynamics, with mainly composed of bioclastic packstone and grainstone. The inter-shoal forms between the shoal of medium hydrodynamics, which is given priority to bioclastic wackestone. The intraplatform shallow is in a lower area with deep water of weak hydrodynamics, dominated by mudstone. (2) On the basis of sedimentation, the restricted platform experiences sea water cementation, selective dissolution and cementation of atmospheric freshwater, and neomorphism during penecontemporaneous period, compaction in the shallow burial period, unselective dissolution of atmospheric freshwater and cementation in the uplift period, burial dissolution and cementation, compaction, pressure dissolving and dolomitization in the medium-deep burial period. (3) The constructive diagenesis, which makes the pore and throat become larger, includes three kinds of dissolution and neomorphism, resulting in intergranular dissolved pore, mould pore and intragranular pore. The destructive diagenesis consists of three kinds of cementation, compaction, pressure dissolving and dolomitization, blocking the primary and secondary pore. The different types of diagenesis have different degrees of and effects on different microfacies, showing polarization characteristics. (4) The bioclastic shoal has a high frequency of exposure. It mainly experiences seawater cementation, neomorphism and three types of dissolution. The primary pore first decreases and then increases, dominated by high-energy sedimentary facies and constructive diagenesis, which forms the medium large pore-middle thin throat reservoirs with middle-high permeability, and it is the main position of high yield wells. The inter-shoal mostly undergoes three kinds of cementation, atmospheric water dissolution, compaction and pressure dissolving, the primary pore first decreases, then increases and finally becomes smaller, it is dominated by middle-low energy sedimentary facies and synthetic diagenesis, resulting in middle pore-micro throat reservoirs with middle-low permeability, and it is the main area of middle yield wells. The intraplatform shallow in diagenetic stage is basically not exposed, mainly experiences three kinds of cementation, compaction, pressure dissolving and dolomitization, the primary pore decreases all the time, controlled by low energy sedimentary facies and destructive diagenesis, which forms the small pore-micro throat interlayers with low permeability, and it is the main region of low yield wells.

References:

Acceptance of Terms and Conditions:
Click here to agree
Corresponding Author(s): didier.lasseux@u-bordeaux.fr

Mass transport combined with heterogeneous reaction in homogeneous porous media is a common process encountered in chemical engineering that is of major concern for many applications ranging from packed bed reactors to porous electrodes. In these systems, reactants are transported by diffusion (and eventually by advection) inside the pores where chemical reactions take place at the solid-fluid interfaces. Modelling the macroscopic behavior of these mechanisms is of prime importance and has been the subject of numerous studies [1, 2, 3, 4]. However, in almost all the analyses reported in the literature, the Kinetic number, Ki, referred to as the ratio between the characteristic time associated to diffusion and the characteristic time associated to reaction at the pore-scale, is considered to be exceedingly small compared to unity. Many industrial processes are indeed operating in this range of Ki, but this constraint is however not always fulfilled. Under these circumstances, the purpose of the present work is focused on the development of macroscopic models in a range of Ki ≲ 1, relaxing the above mentioned restriction.

The study is focused on single-phase transport of a single chemical species undergoing a first-order heterogeneous reaction in rigid and homogeneous porous media. In addition, the advection problem is assumed to be decoupled from the transport/reaction mechanisms. Macroscopic models are derived, with and without advection, using the volume averaging method and the associated closure problems are provided to compute the effective diffusion (or dispersion) and reaction-rate coefficients. In order to elucidate the impact of the Kinetic number on the coefficients involved in the upscaled equations, a Maclaurin expansion in Ki is carried out, yielding models for which the corrections at the successive orders in Ki and the necessary closure problem to compute them are clearly highlighted and numerically solved in periodic unit cells. Validations of the macroscopic models are carried out from comparisons with direct numerical simulations and a discussion is provided on the impact of the corrections. In particular, it is shown that the impact of the Kinetic number is significant on the effective reaction-rate coefficient as well as on the convective macroscopic term in the average transport equation when the Péclet number is non zero but that Ki has a completely negligible contribution to the effective diffusion (or dispersion) tensor.

Keywords: Diffusion, Heterogeneous reaction, Upscaling

References

References:

Acceptance of Terms and Conditions:

Click here to agree
pattern can then be obtained after the withdraw of a liquid phase containing glass beads and con-
fining in an horizontal Hele-Shaw cell, see Knudsen et al., PRE 77, 021301 (2008). What are then the
transport properties within such a geometrical structure? The geometrical constraints with dead-
ends are limiting the transport of diffusing species from a central entry point towards the edges of
the labyrinth. A transient subdiffusive transport can be obtained over a time scale determined by
the wavelength of the pattern.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-C / 622

Digital Material Laboratory: Determination of fractures and frac-
ture networks from X-ray Computed Tomography

David Uribe\textsuperscript{1} ; Holger Steeb\textsuperscript{1}

\textsuperscript{1} University of Stuttgart

Corresponding Author(s): david.uribe@mechbau.uni-stuttgart.de

The study of fractures, fracture networks and especially fracture propagation is of great interest in
rock physiscs and geomechanics. Geothermal and enhanced oil recovery projects rely on the porosity,
permeability and storativity properties of the underground rocks. When a rock has a large number
of fractures, and these interconnect each other, the amount of fluid that can be transported through is
greater as an intact rock or a rock with non-connected fractures. Natural occurring fractures of rocks
from geological processes, which require millennia to occur, usually lead to almost impermeable
rocks, and it is only possible to have fluid flow through major faults. Modern methods to artificially
fracture the rocks rely on pumping large amounts of water into the underground ("hydro-fracking"),
which increases the internal pore pressure in the rocks (reducing the effective stresses) and this
induces the creation of new fractures. This high fluid pressure also allows the natural pre-existing
fractures to propagate.

Although mathematical and numerical models exist for the hydro-mechanical characterization of
single fractures and simple fracture networks, the complexity of the underground rock structure
and local stress state make it difficult for practical technical applications in engineered geosystems.
This limits have been overcome by using large numerical simulations which can more accurately
model the fracture process of rocks, together with the fluid flow process in the microstructure. An
import step of the process requires the validation of the simulations, e.g. the ability of the simulation
to capture more complex process like the creation of secondary tension cracks (wing cracks) from
shear fractures. It is also important to compare the resulting fracture network from experiment with
the predicted one from the simulations.

In the present work, we show the use of a X-Ray micro Computed Tomography (XRCT) system to
determine the geometry of the fractures in porous rocks. One of the limiting factors found in the lit-
erature was the low resolution of the tomograms, and the Poisson noise inherent in CMOS detectors.
Advances in computational power makes it possible to apply advanced noise reduction techniques to
the tomographic sets, and furthermore, apply edge detection algorithms to determine the fractures.
The experiments of rock fracturing include in-situ and ex-situ tensile tests to create wing cracks. A
rock core with an initial fracture was subjected to a shear stress state, where the wing cracks were
created and later on imaged. A second experiment recovers the fracture geometry borehole after
the inner pressure exceed the breakout limit. The last experiment shows the feasibility to image
fracture networks at the near resolution limit of the XRCT system.

References:

Acceptance of Terms and Conditions:
Digital Materials Design

Mark Knackstedt

Corresponding Author(s):

Digital materials design (DMD) coupled with new manufacturing techniques are emerging technologies that have the potential to revolutionize product realization on a global scale. The Economist magazine likened the emergence of these novel imaging, modelling and manufacturing methods to the start of the third industrial revolution. Companies and laboratories now need to turn their attention to detailed multiscale structure, synthesis, processing, properties, and performance characteristics of the materials (most of them porous) that will fundamentally determine the success or failure of direct customised components.

The key to DMD is access to efficient facilities and tools to characterise material structure and function at multiple scales (from nanometers to structural sizes), in multiple states (relaxed vs under compression, before/after reaction or dissolution) and with multiple probes (multiple x-ray spectra, SEM, chemical imaging with infrared spectroscopy, etc.). Experimental data can then be used to support and validate multiscale simulation work within a DMD environment. This talk will first outline the development of an integrated workflow based on 3D multiscale imaging, analysis and modelling for geomaterials. The presentation discusses the potential for the technology to have a much broader reach beyond the geoscience arena—touching companies and industries and giving rise to a wide range of machines, products, or services.

References:

Acceptance of Terms and Conditions:

Poster 2 / 843

Digital Rocks Portal: Curation, Visualization and Analysis of Imaged Porous Materials

Masa Prodanovic¹ ; Maria Esteva¹ ; Richard Ketcham¹

¹ The University of Texas at Austin

Corresponding Author(s): masha@utexas.edu

The Digital Rocks (https://www.digitalrocksportal.org) is the first platform of its kind for data management of images of rock microstructure. It allows preservation, curation, visualization and basic analysis of images of porous materials (and experiments on them). Imaging modalities include X-ray (micro)tomography, (focused ion beam) scattered electron microscopy, optical microscopy, magnetic resonance imaging. We are not limited to imaged data, model media are welcome as well. Any accompanying measurements (porosity, capillary pressure, permeability, electrical, NMR and elastic properties, etc.) required for both validation on modeling approaches and the upscaling and building of larger (hydro)geological models can be associated with images. The portal is implemented within the reliable, 24/7 maintained High Performance Computing Infrastructure supported by the Texas Advanced Computing Center at the University of Texas at Austin.

We overview features of the portal. We create and easy-to-browse presentation of datasets and their inter-relationships, which for 3D datasets includes a movie through the slices, and basic image statistics. We collect information from the user that makes is possible to relate image to the physical sample and its petrophysical properties. Remote visualization through users’ web-browsers is
available on the parallel visualization cluster. All datasets are private (visible only to the author and collaborators) until ready for the public domain. We have a semi-automated publishing pipeline that provides digital object identifiers for cross-referencing in other publications. We continuously improve discoverability, most recently by implementing local search, adding rich snippets to the project metadata, as well as alternative metrics by Altmetrics. Further, we are an approved data repository for Geosciences Data Journal, and are registered in Registry of Research Data Repositories. We are part of EarthCube collaborative to enhance access to Geoscience data, models and resources (https://www.earthcube.org/). As such, we have developed an extensible data model that can be used for linking to other repositories and software.

We finally discuss what it takes to create a go-to benchmark repository for cross-validation and data-driven upscaling (including, but not limited to, machine learning techniques) of microstructure properties in subsurface engineering, material science and geosciences.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 1094

**Dimensionless analysis applied to bacterial chemotaxis towards NAPL contaminants**

Xiaopu Wang¹ ; BEIBEI GAO² ; Roseanne Ford² ; SHUAIWEI GU³ ; WEI ZHONG⁴ ; Kenneth Khaule⁵

¹ China University of Petroleum (East China)
² University of Virginia

Corresponding Author(s): wxp@upc.edu.cn

**Dimensional analysis applied to bacterial chemotaxis towards NAPL contaminants**

Xiaopu Wang 1§, Beibei Gao 2§, Shuaiwei Gu 3, Wei Zhong 1, Kenneth S. Khaule 1, Roseanne M. Ford 2*

1. National Engineering Laboratory for Subsea Equipment Testing and Detection Technology, China University of Petroleum (East China), Qingdao 266555, China
2. Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22904, United States
3. Shandong Provincial Key Laboratory of Oil & Gas Storage and Transportation Security, China University of Petroleum (East China), Qingdao 266555, China

The use of chemotactic bacteria in bioremediation may improve the efficiency and decrease the cost of restoration, which means it has the potential to address environmental problems caused by oil spills. However, most previous studies were focused at the laboratory-scale and there lacks a formalism that can use these laboratory-scale results as input to evaluate the relative importance of chemotaxis at the field scale. Thus, dimensional analysis was adopted to solve this problem. First, the main influential factors were extracted according to the previous researches on bacterial chemotaxis and a set of dimensionless numbers were obtained according to Buckingham theory. After collecting basic parameter values from previous studies, we formulated a dimensionless equation shown as $BR=1.987(P1^{−0.0179})(P2^{−0.3235})(P3^{−0.0319})$, where $BR$ (bacterial ratio) is the ratio of maximum bacteria concentration to its original value, and $P1$, $P2$ and $P3$ are combinations of the derived dimensionless numbers. For $BR$ greater than one, the bioremediation strategy based on chemotaxis is expected to be effective in relative contaminated groundwater system, and chemotactic bacteria are expected to accumulate around non-aqueous phase liquid (NAPL) contaminant sources efficiently.

**Keywords**: Bioremediation; Bacterial chemotaxis; Numerical simulation; Dimensionless analysis

*Corresponding author.

E-mail address: rmf3fl@virginia.edu (R.M.Ford)

§ These authors contributed equally to this work.
Parallel 8-F / 175

Direct experimental measurement of the pair correlation function during the slow drainage of a porous medium

Author(s): Marcel Moura

Co-author(s): Knut Jørgen Måløy ; Eirik Grude Flekkøy ; Renaud Toussaint

1 PoreLab, Department of Physics, University of Oslo
2 CNRS, IPCS UMR 7516, University of Strasbourg

Corresponding Author(s): marcel.moura@fys.uio.no

We have given experimental grounding for the remarkable observation made 30 years ago by Furuberg et al. of an unusual dynamic scaling for the pair correlation function $N(r, t)$ during the slow drainage of a porous medium. The authors of that paper have used an invasion percolation algorithm to show numerically that the probability of invasion of a pore at a distance $r$ away and after a time $t$ from the invasion of another pore, scales as $N(r, t) \propto r^{-1} f (r^D / t)$, where $D$ is the fractal dimension of the invading cluster and the function $f(u) \propto u^{1.4}$, for $u \ll 1$ and $f(u) \propto u^{-0.6}$, for $u \gg 1$. Our experimental setup allows us to have full access to the spatiotemporal evolution of the invasion, which was used to directly verify this scaling [2]. Additionally, we have connected two important theoretical contributions from the literature [3,4] to explain the functional dependency of $N(r, t)$ and the scaling exponent for the short-time regime ($t \ll r^D$). A new theoretical argument was developed to explain the long-time regime exponent ($t \gg r^D$).

References:

Parallel 10-B / 500

Direct numerical simulations of solid particle interactions in suspensions using Smoothed Particle Hydrodynamics

Author(s): Nadine Kijanski

Co-author(s): Holger Steeb

1 University Stuttgart
2 University of Stuttgart

Corresponding Author(s): nadine.kijanski@mechbau.uni-stuttgart.de

Suspensions and their applications can be found in many fields of mechanical, civil and environmental engineering. The rheological behavior of suspensions strongly depends on the concentration
of suspended particles. To consider the flow behavior as well as fluid-solid interactions in dilute suspensions, we present 3D Direct Numerical Simulations (DNS) of a single-phase fluid with discrete embedded solid particles. We therefore present an implementation using the general-purpose particle simulation toolkit HOOMD-blue [1, 5] extended for the usage of Smoothed Particle Hydrodynamics (SPH) [2, 5]. Since both the fluid and the solid phase is discretized by particles, SPH as a Lagrangian particle method presents a good choice to model this particular non-linear problem. The advantages of DNS with SPH compared to often used coupled SPH-DEM approaches are the fully resolved solid-fluid interfaces and the here acting hydrodynamical forces. Solid-solid contact and resulting interaction forces are included into the model by using a simplified Hertz-Mindlin contact model [4]. The model is applied on all solid particles representing the solid phase in the suspension. Thus, in case of contact, an additional particle force is added to the prescribed forces in the local momentum conservation equation. We are aiming for a discussion about the validity of the implementation. Thus numerical investigations include simulations with fully elastic collisions with and without a surrounding solvent as well as free falling of a solid grain with and without a surrounding fluid. To review the results of the approach, we finally discuss an example with multiple spherical solid grains in a single-phase fluid in different configurations as for example gravity or parallel flow. Resulting local particle properties as velocity and shear stresses are considered and compared to known analytical solutions. We focus on particle scale effects as for example the mobilization forces acting on a bed of solid grains and the resulting transport of single particles as well as the transformation of flow behavior, for example the evolution of shear flow, dependent on the number of suspended particles.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-E / 910

Direct observation of phase change in sub-10 nm porous media

Arnav Jatukaran1 ; Junjie Zhong1 ; Aaron Persad1 ; Ali Abedini1 ; Atena Sharbatian1 ; Yi Xu1 ; Farshid Mostowfi2 ; David Sinton1

1 University of Toronto
2 Schlumberger-Doll Research

Corresponding Author(s): arnav.jatukaran@mail.utoronto.ca

Phase change at the nanoscale is critical to many industrial applications including rapidly emerging unconventional oil and gas production from nanoporous shale reservoirs. The thermodynamic behaviour of hydrocarbons confined to these nanopores is expected to deviate significantly from bulk properties and there is little experimental data to validate theories. This research aims to visually observe the evaporation of hydrocarbons in a nanofluidic chip that accurately represents the geometric dimensions and the pressure/temperature conditions observed in shale. The chip consists of a nanoporous network of two-dimensional (2D) nano pores with dimensions down to 8 nm. Using
an experimental procedure that mimics pressure drawdown during shale oil/gas production, our results show that evaporation of pure propane takes place at pressures lower than predictions from the Kelvin equation (maximum deviation of 11%). We probe evaporation dynamics as a function of superheat and find that vapor transport resistance dominates evaporation rate. For the transport resistance in the sub-10 nm nanoporous media, the contributions of the Knudsen flow and the viscous flow are found to be approximately equivalent. We also observe a phenomenon in sub-10 nm confinement wherein lower initial liquid saturation pressures trigger discontinuous evaporation resulting in faster evaporation rates. Additionally, we also extend this work to study evaporation and cavitation dynamics in nanofluidic devices with (a) mixture of pore sizes coupled with (b) mixture of hydrocarbons. Collectively, the results presented will aid in increasing the efficiency of shale production and will inform modelling and simulation of shale gas production.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-D / 628

Direct observation of the moisture distribution in castables at high temperatures as studied by NMR

Leo Pel1 ; Ahmed Barakat2 ; Olaf Adan1

1 Eindhoven University of Technology
2 Eindhoven University of Technology

Corresponding Author(s): lpel@tue.nl

In this study, the drying behavior for a variety of calcium alumina- and hydratable alumina-bonded refractory castables was investigated in the temperature regime of first-drying, i.e., up to 300 °C. Using a specialized high-temperature Nuclear Magnetic Resonance (NMR) setup, we were able to directly and non-destructively measure the spatially and temporally resolved moisture distribution, while simultaneously measuring the temperature distribution as well. We employ a high-temperature correction scheme that calibrates the effects of the surface relaxation for rising temperatures. This setup makes use of a high-sensitivity Birdcage-coil for measuring the quantitative moisture content at high-temperatures, while also utilizing a mini-coil for calibrating relaxation changes, as a function of temperature and hydration state, taking place in the sample throughout a drying experiment. These measurements give for the first time a direct insight into the drying behaviour of castables and show that the drying front speed and temperature are strongly correlated with control of key material parameters such a as binder content and water demand. In addition these measurements provide a direct insight into the steam pressures which are generated within the samples and hence in the risk of explosion.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-H / 1128

Direct pore-scale two-phase transport simulation with interface transfer

Julien Maes1

1 Heriot-Watt University
Corresponding Author(s): j.maes@hw.ac.uk

Multiphase multispecies transport is an essential field of studies for a wide range of engineering applications including acid gas treatment, waste water management and bubble column reactor. In particular, pore-scale investigations of subsurface processes have recently attracted a lot of attention in many domains such as oil and gas production, CO2 storage and contaminant hydrology. On the one hand, pore-scale experimental techniques allow a direct visualization of the different processes involved in 2D micromodels or in 3D rocks. On the other hand, pore-scale numerical models allow the mixing of phase and chemical species to be resolved on a pore-by-pore level. Numerical investigation of interfacial mass transfer can be done using Direct Numerical Simulation (DNS) of the Navier-Stokes Equation (NSE). DNS of two-phase flow can be performed using the Volume-Of-Fluid (VOF) method. VOF methods have been successfully applied to complex two-phase processes such as drainage and imbibition in complex 2D and 3D porous media. However, extending this work to multiphase multispecies transport in such complex porous media has proven to be a real challenge. One of the reason for this is the difficulty to transport a concentration field in the domain while insuring the continuity of fluxes and chemical potentials at the fluid/fluid interface. The objective of this work is to present a review of recent advancements in this domain, which allow us, for the first time, to simulate multiphase multispecies transport with the VOF method for a wide range of flow regime.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 318

Direct sampling versus a new multiphase-multiresolution simulated annealing approach: Which porous media reconstruction algorithm performs best?

Author(s): Laurent Lemmens¹

Co-author(s): Bart Rogiers²; Eric Laloy²; Mieke De Craen²; Diederik Jacques²; Rudy Swennen³; Guillaume Desbois⁴; Janos L. Urai⁴; Marijke Huysmans⁵

¹ Ku Leuven / SCK-CEN
² SCK-CEN
³ KU Leuven
⁴ RWTH Aachen University
⁵ Ku Leuven

Corresponding Author(s): laurent.lemmens@sckcen.be

The microstructure of a radioactive waste confinement barrier strongly determines its flow and transport properties. Numerical flow and transport simulations for these porous media at the pore-scale are necessary for in-depth understanding of the pore-scale processes, and might for instance allow making predictions beyond current experimental timescales. Such simulations of course require input data that describe the microstructure as accurately as possible. This data can be deduced from various imaging techniques, but for complex porous materials with heterogeneities at different spatial scales, a combination of imaging techniques is required. To merge all available information into a single synthetic but realistic microstructure, and to lower the need for e.g. costly 3D imaging, high quality numerical reconstruction algorithms are needed.

Simulated annealing (SA), which is based on structural descriptors, is one of the oldest approaches and has recently received renewed attention. The method is typically only applied to binary images and is computationally very demanding without optimized algorithms and inventive computational approaches. We extended the state-of-the-art of the SA approach to multiphase reconstructions in a multiresolution-multiphase hierarchical approach, which allow for decreasing the computational burden. The algorithm reconstruct first a binary image at a coarse resolution with refinement afterwards. Once the simulation of the first phase is finished, the corresponding pixels are frozen and
the next phase is reconstructed. This new methodology reduces the computational time by at least 50% compared to single grid simulations while additionally improving the reconstruction quality. In reconstruction with a high-particle-size-to-simulation-grid-dimension ratio, the speed up can be several orders of magnitude.

Compared to Direct Sampling (DS), the new SA algorithm does not show the problem of honouring the histogram and the occurrence of verbatim copies. Additionally, the new SA algorithm shows an improvement in the long range connectivity of the different phases within the training image. We show this using two case studies: cement paste and Boom Clay.

References:

Acceptance of Terms and Conditions:
Click here to agree

---

**Poster 2 / 945**

**Direct simulation of permeability including Klinkenberg effect**

Ganapathi Balasubramanian\(^1\); Chaitrali Ghodke\(^2\); David M. Freed\(^3\); Bernd Crouse\(^4\)

\(^1\) Exa
\(^2\) Exa Corporation

**Corresponding Author(s):** bernd.crouse@3ds.com

Core analysis for characterization of rock properties such as permeability involves laboratory flow experiments performed at lower temperature and pressure than the conditions typically present in subsurface hydrocarbon reservoirs. For gas permeability in particular, slippage flow can occur at reservoir conditions, resulting in higher apparent permeabilities than would occur for Darcy flow. Known as the Klinkenberg effect, the impact on permeability can be significant, and depends on the gas type and characteristic pore sizes that govern the fluid flow; the pore sizes in turn depend on the formation rock matrix and may also be influenced by effective stress and clay content.

Digital rock physics has emerged over the last decade as a complimentary or alternative technique to laboratory testing for rock property characterization. In this study, we perform direct numerical simulation of gas flow in porous media over a wide range of Knudsen number regimes, where the dimensionless Knudsen number is given by the fluid particle mean free path divided by a characteristic channel width for the porous medium. As Knudsen number increases, the ratio of apparent permeability to Darcy permeability (S) increases as the system moves from Darcy flow to slip, transition, and finally the Knudsen flow regime, as seen in the included Figure. This study uses a flow simulator based on the Lattice Boltzmann Method (LBM) technology. First the simulator is benchmarked by comparing predicted results to existing experimental data over the full range of Knudsen number flow regimes ranging from 0.001 to 10 for flow in rectangular channels (Ewart et al. and Colin et al.) and 3D micro-tubes (Perrier et al.). Resolution studies show that the flow simulations retain good accuracy at low grid resolutions which are typically required for digital rock based analyses. Next, simulations are performed to demonstrate the Klinkenberg effect in tight sandstones and unconventional shale rocks. It is shown that the apparent permeability of tight rocks can be up to 2 orders of magnitude higher than would occur for Darcy flow, which corresponds to the unexpectedly high permeabilities sometimes observed in the field.

References:


Acceptance of Terms and Conditions:
**Poster 2 / 301**

**Direction Dependency of Relative Permeability for Oil-Water Two Phase Flow in Vugular Porous Medium**

Shihan SONG¹ ; Yuan DI¹ ; Shuyue CUI² ; Zhijiang KANG²

¹ Peking University  
² Exploration & Production Research Institute, SINOPEC

**Corresponding Author(s):** 1501111645@pku.edu.cn

Multi-phase flow process in porous medium are generally simulated with introduction of relative permeability, which is assumed to be a scalar function of phase saturation. Previous research have demonstrated this assumption might not be suitable for capillary force dominated heterogeneous porous medium. Similarly, in vugular porous medium, the free flow region in vugs would introduce vertical velocity component, causing the flow field to differ. Two-dimensional experiments are conducted to examine such effect. The physical model are artificial homogenous and isotropic porous medium square plates, and vugs are designated as cylindrical holes. A group of models with axisymmetric vug distribution are designed so that the fluid flow in two principal directions are the same if the plate is placed horizontally but different if the plate is placed vertically. Also for general purpose another group of models with random placed vugs are designed to simulate actual reservoirs. The upscaled relative permeability curves in two principal directions are measured and compared. Supplemental numerical simulation are also conducted on two simulators. The first is a finite volume simulator KarstSim with the assumption of gravity segregation and instantaneous establishment of steady-state in vugs, the second is a commercial finite element software. The experiment result indicates that the direction of upstream fluid flow have a significant influence on the flow field within the physical model, and is presented in the relative permeability curves. This effect is pronounced in the cases where the vugs are distributed in specific orders. The numerical result are in good agreement with the result of experiments. Based on the results, we prompt the need to introduce a secondary variable in the relative permeability function, which is the angle between the upstream flow direction and the vertical direction to better simulate the multi-phase flow process in vugular porous medium.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

**Parallel 8-C / 253**

**Discontinuous Galerkin approximation of flows in fractured porous media on polytopic grids**

Chiara Facciola¹ ; Paola Antonietti¹ ; Marco Verani¹ ; Alessandro Russo²

¹ MOX Politecnico di Milano  
² Università di Milano Bicocca- IMATI CNR Pavia

**Corresponding Author(s):** chiara.facciola@polimi.it

We propose a new formulation based on discontinuous Galerkin (DG) methods in their generalization to polytopic grids for the simulation of flows in fractured porous media. The method that we propose is very flexible from the geometrical point of view, being able to handle meshes made of arbitrarily shaped elements, with edges/faces that may be in arbitrary number (potentially unlimited)
and whose measure may be arbitrarily small. Therefore, our approach is very well suited to tame the geometrical complexity featured by most of applications in the computational geoscience field, such as petroleum engineering, nuclear waste storage, geothermal energy, etc. More precisely, we adopt a model for single-phase flows, that is valid for fractures with both large and low permeability. This model considers the case of a single fracture, treated as a (d -1)-dimensional interface between two d-dimensional subdomains, \( d = 2, 3 \). The flow in the porous medium is assumed to be governed by Darcy’s law and a suitable reduced version of this law is formulated on the surface modelling the fracture. Physically consistent coupling conditions are added to account for the exchange of fluid between the fracture and the porous medium. We focus on the numerical approximation of the coupled bulk-fracture problem, employing Discontinuous Galerkin finite elements on polytopic grids. The choice of DG methods arises spontaneously in view of the discontinuous nature of the solution at the matrix-fracture interface. However, this is not the only motivation. Indeed, the interface conditions can be naturally formulated using jump and average operators and embedded in our variational formulation, so that DG methods turn out to be a very powerful approach for handling the (weak) coupling of the two problems. We theoretically analyze our discrete formulation, prove its well-posedness and derive optimal a priori error estimates in a suitable (mesh-dependent) energy norm. Finally, we consider both benchmark test cases with analytical solution and a realistic example driven by petroleum engineering applications, namely the quarter five-spot problem. We demonstrate that our scheme can efficiently handle both situations.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 6·F / 164

Discrete-continuum multiscale model for evolving microaggregates in porous media

Andreas Rupp\(^1\); Nadja Ray\(^1\); Alexander Prechtel\(^1\); Peter Knabner\(^1\)

\(^1\) Friedrich-Alexander University Erlangen-Nürnberg

Corresponding Author(s): andreas.rupp@fau.de

Microaggregates are the fundamental building blocks of soils and thus important for its structure, properties and functions [Totsche et al]. Although there has been much research on the links, dynamics, stability, and structure of soil microaggregates, there is still a substantial lack of quantifying the relationships between the key factors of their dynamics. Those key factors are soil fauna, microorganisms, roots, inorganics, and physical processes [Totsche et al]. We assess the complex coupling of biological, chemical and physical processes at different scales with the help of a mechanistic modelling approach in order to gain a model-based mechanistic understanding of the formation, build-up, composition, properties and stability of microaggregates.

Our dynamic framework combines biomass development and structural changes in the solid originating from stabilizing sticky agents or electric effects in a comprehensive micro-macro model [Ray et al]. It uses a versatile discrete cellular automaton method (CAM) on the microscale with a continuous PDE formulation on the micro and the macroscale [Ray et al]. This means that the underlying time-dependent computational domain for the pore scale, i.e. the distribution of a solid, biomass, a wetting, and a non-wetting fluid is determined discretely by means of a CAM. The diffusion of mobile bacteria, possibly transforming into immobile biomass, nutrients, and ions are prescribed by means of PDEs, likewise, the surface concentration of a sticky agent tightening together solid or bio cells (in the cellular automaton context) is considered. The idea of using a CAM setting with biofilm growth at the pore scale goes back to work in [Tang / Valocchi, Tang et al].

To omit the explicit tracking of interfaces as it is necessary in level-set approaches we use this combined discrete-continuum approach. As the soil is evolving in this setting we have to use a discretization for the PDE systems in the fluid that is robust and handles discrete discontinuities. The local discontinuous Galerkin (LDG) method is suitable for this task.
One main objective of this research is to examine the strong interplay between functional properties and geometric structure. To that end standard homogenization results are used to compute the soil’s characteristic properties such as porosity or effective diffusion tensors for the resulting complex and time-dependent geometries.

Exemplarily we show how structure formation can be studied with the help of simulations by focussing on isolated mechanisms, e.g. different ranges of attracting forces or varying size of building units. Simulations also complement aggregation experiments for goethite and ille with EPS and address questions of homoaggregation, and heterooaggregation of different particles, also investigating the influence of extracellular polymeric substances stemming from microorganisms.

References:
Click here to agree

Poster 3 / 812

Discriminative Random Field Models for Subsurface Source Zone Characterization and Uncertainty Quantification

Masoud Arshadi¹ ; Linda Abriola¹ ; Eric Miller¹ ; Clara De Paolis Kaluza²

¹ Tufts University
² Northeastern University

Corresponding Author(s): masoud6a@gmail.com

Application of flow and transport simulators for prediction of the release, entrapment, and persistence of dense non-aqueous phase liquids (DNAPLs) and associated contaminant plumes is a computationally intensive process that requires specification of a large number of material properties and hydrologic/chemical parameters. Given its computational burden, this direct simulation approach is particularly ill-suited for quantifying both the expected performance and uncertainty associated with candidate remediation strategies under real field conditions. Prediction uncertainties primarily arise from limited information about contaminant mass distributions, as well as the spatial distribution of subsurface hydrologic properties. Application of direct simulation to quantify uncertainty would, thus, typically require simulating multiphase flow and transport for a large number of permeability and release scenarios to collect statistics associated with remedial effectiveness, a computationally prohibitive process.

The primary objective of this work is to develop and demonstrate a fast and effective methodology that employs measured field data to produce equi-probable stochastic representations of a subsurface source zone that capture the spatial distribution and uncertainty associated with key features that control remediation performance (i.e., permeability and contamination mass). Here we employ probabilistic models known as discriminative random fields (DRFs) to synthesize stochastic realizations of initial mass distributions consistent with known, and typically limited, site characterization data. Using a limited number of full scale simulations as training data, a statistical model is developed for predicting the distribution of contaminant mass (e.g., DNAPL saturation and aqueous concentration)
across a heterogeneous domain. Markov chain Monte Carlo (MCMC) sampling methods are then employed, in conjunction with the trained statistical model, to generate realizations conditioned on measured borehole data. Performance of the statistical model is illustrated through comparisons of generated realizations (metrics) with the 'true' numerical simulations. Finally, we demonstrate how these realizations can be used to determine statistically optimal locations for further interrogation of the subsurface.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-C / 590

Dispersion in Hyperporous Fractures: Surface Properties and Scaling

Bowen Ling1; Alexandre Tartakovsky2; Ilenia Battiato1

1 Stanford University
2 Pacific Northwest National Laboratory

Corresponding Author(s):

Permeable and hyperporous surfaces are common in natural systems, such as fractured rocks. Flow and transport above such surfaces is significantly affected by the surface properties, e.g., matrix porosity and permeability. However, the relationship between such properties and macroscopic solute transport is largely unknown. We focus on mass transport in a two-dimensional fracture with permeable porous walls under fully developed laminar flow conditions. By means of perturbation theory and asymptotic analysis, we derive the set of upscaled equations describing mass transport in the coupled fracture-permeable matrix system and an analytical expression relating the dispersion coefficient with the properties of the surface, namely porosity and permeability. Our analysis shows that their impact on dispersion coefficient strongly depends on the magnitude of Peclet number, i.e., on the interplay between diffusive and advective mass transport. Additionally, we demonstrate different scaling behaviors of the dispersion coefficient for thin or thick porous matrices. Our analysis shows the possibility of controlling the dispersion coefficient, i.e. transversal mixing, by either active (i.e. changing the operating conditions) or passive mechanisms (i.e. controlling matrix effective properties) for a given Peclet number. This work lays the foundation to understand the impact of matrix permeability on transport in fractures. The proposed upscaled model is validated against microfluidic experiments.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 238

Dissipative Particle Dynamics Based Mesoscale Modeling of Multiphase Flow in Reconstructed High-Resolution Nanoporous Shale Pore Networks

Yidong Xia1; Jan Gora2; Zhen Li1; Lixiang Luo1; Hai Huang3; Milind Deo2; Matthew Andrew5

1 Idaho National Laboratory
2 University of Utah
Numerical modeling has been an increasingly important approach for better understanding fluid flow and transport phenomena in organic-rich, nanoporous shale. However, deployment of numerical models in the context of nanoporous shale is challenging because of the multi-length-scale nature of the porosity in shale, where pore sizes can range between the nanoscale (~10^{-9} m) and microscale (~10^{-6} m), because of the complex physical and chemical interaction between fluid and wall surfaces in pores, and because of the demanding computing costs required for simulations to reach the desired spatial and temporal scales. For example, simulations of pore-network fluid flow in a representative region of interest (ROI) in a micro core sample are beyond the current computational limit of the molecular dynamics models, and also immature with the particle-differential-equations based continuum computational fluid dynamics models. The class of dissipative particle dynamics (DPD) models, which were originally introduced for the modeling of microscopic hydrodynamics, have recently been extended and applied for mesoscale flow and transport in porous media. A remarkable feature of the DPD models is that they are able to reproduce some of the key characteristics of fluids at both the molecular and continuum scales, which make these models more flexible for modeling multi-length-scale fluid systems. Among the many variances of DPD models, the many-body DPD (mDPD) model has demonstrated particular suitability for modeling pore-network flow and transport. In the authors’ earlier work [Xia et al., 2017, *Physics of Fluids* 29(5)], a modeling & analysis workflow that integrates the digital rock physics to a parallel mDPD code was developed for simulating multiphase flow in shale, where a focused ion beam scanning electron microscope (FIB-SEM) digital imaging process is used to provide voxel data to inform the construction of wall surfaces of the connected pores in the simulations. In the present work, an improved mDPD model for the workflow will be presented, in which an enhanced non-/partial-slip boundary condition algorithm [Li et al., 2017, *Journal of Computational Physics*] will be applied for better resolving wall-fluid interactions in the multiscale pore networks of shale. Moreover, in order to reduce load imbalance in parallel computing with massive CPU nodes and hence realize the mDPD flow simulations in shale ROIs at a desirably larger spatial and temporal scale, a node-level multithreading parallelism will be implemented in our MPI parallel mDPD code, and deployed along with a recursive coordinate bisection (RCB) based adaptive domain repartitioning algorithm. Simple flow simulations in manufactured slit nanopores will be presented for verification and validation of the improved workflow. Multiphase flow simulations that contain hundreds of millions of mDPD particles will then be presented for permeability-fluid dependence study in the reconstructed high-resolution nanopore networks of a selected shale ROI. Simulation results and computational performance will be reported and analyzed. The workflow developed in the present study is still relatively new in the area of virtual rock analysis, especially for nanoporous shale. Nevertheless, it is being continuously improved toward a robust and accurate mesoscale model that is expected to bridge the gap between its molecular- and grain-scale counterparts.

References:


Click here to agree

---

**Dissipative Processes during Two-Phase Flows**

Sophie Roman\(^1\); Cyprien Soulaine\(^2\); Anthony Kovscek\(^2\)

\(^1\) *Institut des Sciences de la Terre d’Orléans*

\(^2\) *Stanford University*
Corresponding Author(s): sophie.roman@univ-orleans.fr

A fundamental understanding of multiphase flows in porous media is relevant to enhanced oil recovery as well as to the process of CO2 sequestration in hydrocarbon reservoirs and saline aquifers. Recently, we quantified two-phase flow mechanisms in micromodels that represent the pore networks of natural complex porous media [1]. Using micro-Particle Image Velocimetry (micro-PIV), we are able to measure accurately the velocity distributions in porous media with a typical pore size of 5-40\(\mu\)m. Moreover, we observe and quantify dissipative events, such as eddies within the aqueous phase [1]. These observations motivated further measurement of interfacial dynamics as well as pore-scale and thin film hydrodynamics [2] in a two-phase flow setting. Following our initial work and [3], [4], [5], we explore the origins of dissipative processes at pore scale and their consequences on the upscaling of rock and fluid properties, i.e. relative permeabilities. For that purpose, we performed microfluidics experiments using porous media of varying complexity. Microfluidic experiments provide direct observations of dissipative events happening at pore scale. These experiments are associated with image processing techniques to track the fluid/liquid interface, to measure velocity distributions as well as thin film dynamics. We provide quantitative data on dissipative events, i.e. the trapped wetting phase showing a recirculating motion, for various flow conditions, with the aim to aid interpretation of core-scale relative permeability.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-H / 141

Dissolution patterns and rates in a heterogeneous limestone studied by using a multicomponent reactive transport model at the pore scale

Apoorv Jyoti\(^1\); Ralf R. Haese\(^2\)

\(^1\) PhD Student
\(^2\) Professor

Corresponding Author(s): ajyoti@student.unimelb.edu.au

Reactive transport modelling at the pore scale explores the spatial-temporal changes in the pore network geometry, the flow field and water composition at sub-centimetre scale. It requires a true representation of fluid-mineral boundaries and their role as zones of fluid-mineral reactions, spatially explicit mass transport and a set of chemical equations to calculate the aqueous speciation and rate of reactions.

We developed a 3D multicomponent reactive transport model by coupling the transport equation solver COMSOL to the geochemical reaction solver iPHEREQC C++ (Parkhurst and Appelo 2013) library using the java-based COMSOL-PHREEQC interface, iCP (Nardi, Idiart et al. 2014). A particular feature of the model is the implementation of the fluid-mineral boundary layer where kinetically controlled mineral dissolution and precipitation can occur.

Flow-through experiments were carried out to study the dissolution of a small bioclastic limestone core from Mt. Gambier, South Australia, through the injection of an acid. The time-dependant pore network geometry of the sample was derived from microCT images and the water composition continuously monitored throughout the experiment. Excellent agreement was found for the whole-core dissolution rate derived from the image-based change in volume fraction, the quantification of dissolved calcium in the outflow and the 3D reactive transport model. Acid buffering through carbonate dissolution strongly controls the dissolution pattern: A high degree of face dissolution as
opposed to wormhole formation is observed in sequential microCT images and simulation results. Our study highlights the need to include the aqueous chemical system in reactive transport modelling in order to predict the dynamic changes in dissolution rates and the associated changes in the pore geometry.

References:


Click here to agree

Poster 2 / 71

Doping SBA-15 with Nickel Oxide by Freeze-Drying Impregnation

Albert Praise1, Jens Meissner1, Reinhard Schomäcker1, Gerhard Findenegg1

1 Technical University Berlin

Corresponding Author(s): findenegg@chem.tu-berlin.de

Immobilization of transition metal oxides on a solid support by impregnation with solutions of metal salts is a common route in catalyst design. An inherent difficulty of such methods is that precipitation by solvent evaporation leads to undesirably large catalyst crystallites forming at the outer surface of the porous support. In this study we explore the potential of an alternative route, based on eutectic crystallization of the aqueous metal salts in the pores of ordered mesoporous silica and removal of ice by freeze-drying. The so-called two-solvents method was used to selectively load the pore space [2], i.e., to avoid an excess layer of salt solution coating the outside of the silica particles. The resulting samples were frozen with liquid nitrogen and lyophilized, then slowly heated to 500°C and calcined. A morphological and structural analysis of the formed nickel oxide species in the pores was performed and compared to samples prepared by conventional solvent evaporation. The immobilized nickel oxide prepared by the new technique appeared in two morphologies: (a) crystallites of size somewhat smaller than the pore diameter of SBA-15 (7 nm); (b) material causing no XRD reflections but still detectable by energy-dispersive X-ray spectroscopy (EDX). Nitrogen sorption isotherms provided further information about the distribution of NiO in the pores: For samples containing NiO crystallites the pore-size distribution (psd) of the primary pores was strongly broadened towards lower diameters. For samples showing no crystallites the psd remained narrow but was shifted, indicating that NiO was forming a thin layer at the pore wall.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 791
Droplet Flow Regimes in a T-Section Microchannel: Assessment of Volume of Fluid Formulations

Saideep Pavuluri¹; Julien Maes¹; Florian Doster¹

¹ Heriot-Watt University

Corresponding Author(s): f.doster@hw.ac.uk

Keywords:
Droplet flow regimes, Interfacial dynamics, Volume of Fluid method, Parasitic currents, Direct Numerical Simulations

Abstract:
Multiphase flow in microfluidic devices that produce identical droplets/bubbles at a known frequency has gained attention due to its use in biomedical, chemical and engineering applications.

In this numerical study, we investigate the flow dynamics in a 2D ‘T’ shaped microfluidic channel where two fluids (wetting and non-wetting) are injected orthogonally and meet at a junction. We use Direct Numerical Simulations (DNS) with the Volume of Fluid (VoF) method where the fluids are distinguished based on a volumetric colour function. DNS-VoF captures the topological changes (ex: pinch-off of an interface) automatically, unlike other methods (ex: Front-tracking) which require manual interventions.

However, Parasitic currents (PC) around the interface potentially occur due to inaccurate computations of the capillary force $F_c$. The Continuum Surface Force (CSF) [3] expresses $F_c$ in a simplistic manner. However, the capillary terms are imprecise and show larger PC. To reduce PC, several formulations are available, such as Sharp Surface Force (SSF) [2, 3] and Filtered Surface Force (FSF) [3]. These formulations advect the interface numerically while trying to retain a sharp interface. Alternatively, Piecewise Linear Interface Construction (PLIC) [4], geometrically constructs and advects the interface. Height functions are used to increase the order of accuracy in computing $F_c$.

Though a number of DNS-VoF validations with experiments and analytical models are available [5], a systematic investigation of the potential impact of PC on the droplet formation (possibilities of initiating a premature break-up or skipping pinch-off) and on the droplet length for a wide range of capillary number are still not available. Indeed, our numerical simulations show different flow regimes in the microchannel using the above mentioned VoF formulations for the same flow conditions. Further, when there is a pinch-off, the length of the droplet formed also varies for different VoF formulations. To validate the accuracy of the numerical solvers we make use of a solution that can be derived using geometrical and force balancing techniques.

References:


Click here to agree

Parallel 9-B / 520
Droplet Impact on Fabric

Thijs de Goede$^1$; Stefan Kooi$^1$; Ali Mazloomi$^2$; Dominique Derome$^3$; Jan Carmeliet$^2$; Noushine Shahidzadeh$^4$; Daniel Bonn$^3$

1 University of Amsterdam
2 ETH Zurich
3 Empa
4 University of Amsterdam - Institute of Physics

Corresponding Author(s): t.c.degoede@uva.nl

Although droplet spreading on smooth surfaces is well known, spreading on textile materials is still not fully understood. Compared to a solid surface, on textile the liquid can penetrate the holes in the fabric but also spontaneously flow through the porous networks inside the fabric (wickimg), making droplet spreading more complex compared to smooth surfaces. Understanding droplet spreading on textile materials is important for applications in the textile industry and forensic research.

We study droplet impact on thin monolament polyester fabric as a function of the fabric pore size and its wettability. First, the difference between droplet spreading on a smooth surface (stainless steel) and the fabric is investigated where the fabric is either placed on a substrate or suspended in the air. We show that a droplet spreads less on the fabric compared to the smooth surface. Furthermore, a difference in spreading is observed between the spreading on fabric with and without substrate due to the liquid penetrating the fabric. Secondly, droplet fragmentation of the penetrating liquid is investigated. Using simulations, we determine the physical processes behind droplet spreading and the subsequent fragmentation.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 1-F / 574

Droplet impact and penetration on porous stones

Amir Ashrafi Habibabadi$^1$; Vontobel Peter$^2$; Dominique Derome$^3$; Jan Carmeliet$^1$

1 PhD student at Department of Mechanical Engineering, ETH Zurich
2 Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut (PSI)
3 Empa
4 ETH Zurich

Corresponding Author(s): dominique.derome@empa.ch

Droplet impact on porous surfaces is a phenomenon of interest in several applications and is studied here in the context of wind-driven rain impacting building facades. The aim of the this work is understanding and controlling the droplet dynamics and penetration into the porous surface. Despite of the wide applications of this phenomenon, the studies in this field are mostly limited to the impact on impermeable surfaces so far.

During a heavy rain event, more and more droplets hit a porous surface, spread and get adsorbed. At some point, the porous material is saturated at its surface and the subsequent water droplets will lead to a water film to form on the surface [1]. This phenomenon is studied in this work in detail for different porous stones. The rain event is simulated using a train of droplets impacting at the same place, with definite time intervals. The water distribution inside the porous samples is obtained
using neutron imaging at the Neutra beamline of the SINQ at Paul Scherer Institute (PSI), Villigen, Switzerland and the droplet impact dynamics is captured using shadowgraphy imaging with high speed camera. These two informations are combined together to understand the relation between the droplet spreading behavior, the moisture content at the surface and the water distribution within the porous stones during the train of impacting droplets. It is found that the droplet spreading ratio increases with increasing surface moisture content, however this increment is different for each stone, depending on porosity, and pore size distribution, surface tension effects and energy dissipation on the wetted surface. An energy balance model for droplet impact on porous surfaces is proposed and the effect of moisture distribution inside the material on droplet spreading is determined. The model is compared with the experimental results showing good agreement. Moreover, the movement of wetting front inside the material is studied using the neutron images. It is seen that the water penetration into the stones depends mainly on impact velocity, but also a role of stone characteristics is identified. The water distribution inside the material cannot be considered neither as resulting from a uniform source, nor a point source.

References:


Click here to agree

Poster 4 / 490

Drying characteristics of polydisperse particle aggregates in the capillary-dominated regime

Son Thai Pham1 ; Bruno Chareyre 2 ; Evangelos Tsotsas3 ; Abdolreza Kharaghani4

1 Thermal Process Engineering, Otto von Guericke University
2 SSRS, University Grenoble-Alpes; SSRS, CNRS
3 Otto-von-Guericke University
4 Otto von Guericke University

Corresponding Author(s): abdolreza.kharaghani@ovgu.de

In this study, a discrete pore-scale model is developed to predict the drying characteristics of an aggregate composed of primary particles with a multimodal size distribution. The solid phase is represented by a cubic particle packing and the complementary pore space is constructed by using the pore-scale finite volume approach. The vapor forming as a result of (slow) evaporation escapes through the top surface of a porous particle aggregate. A drying algorithm is implemented that takes into account the formation of liquid clusters and which is based on the combination of the classical invasion percolation algorithm, applied to each cluster, and the computation of the evaporation rate for each cluster. Both capillary liquid flow and vapor diffusion are obtained from a pore-scale finite volume model. Taking a regular mono-sized particle aggregate as a reference, the size and spatial distributions of the primary particles are systematically varied to represent the change in the corresponding void space structure. The simulation results indicate the impact of the spatially correlated pore-scale heterogeneity on the drying kinetics of these particle aggregates. This work is our first step towards simulating the complex thermo-mechanical behavior of particle aggregates during drying.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 43
Drying regimes in homogeneous porous medium from macro to nano-scale

Author(s): Philippe Coussot

Co-author(s): Stéphane RODTS ; Dave WEITZ ; Jules THIERY

1 Univ. Paris-Est
2 Harvard University
3 Harvard Univ.

Corresponding Author(s): philippe.coussot@ifsttar.fr

From MRI visualization of internal liquid distribution in time during convective (given air flux) drying of uniform bead packings with pore size from micro- to nano-meter, we show that, at first sight, the standard regimes of drying may be observed in any case: first a constant drying rate regime (CRP) associated with a homogeneous desaturation, followed by a falling rate period (FRP) associated with the growth of a dry region from the sample free surface, and during which the drying rate varies in accordance with vapor diffusion through the dry porous region. However several more original phenomena can be highlighted: 1) the duration of the CRP decreases when the pore size decreases (for a given air flux); 2) for pore size below say a few tenth of nanometers, despite an apparent homogeneous desaturation the drying rate continuously decreases, a phenomenon likely due to Kelvin effect; 3) at any time in the FRP the material still desaturates homogeneously in the wet region (below the dry region), which suggests the existence of continuous liquid flow towards the interface of higher evaporation, even for very low saturation or very small pore size. However, in the latter case, it appears that the corresponding net flow rate is almost independent of the pore size, an effect which cannot be described by a model based on a simple Darcy’s law model with capillary effect as the driving force, which gives a scaling with the pore size. Instead it is likely that, paradoxically, even if this net flow is unidirectional and capillary driven, it is again governed by a series of diffused local capillary equilibrations throughout the sample, leading to a net liquid transport with a specific dynamics almost independent of the pore size.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 463

Dynamic phase connectivity in pore-network models

Author(s): Dmytro Petrovskyy

Co-author(s): Rink van Dijke ; Zeyun Jiang ; Sebastian Geiger ; Tianshen Huang

1 Heriot-Watt University

Corresponding Author(s): dop1@hw.ac.uk

Pore-network modelling is an efficient method to simulate pore-scale multi-phase flow. The pore-network consists of a collection of idealized interconnected discrete network elements – pore nodes and pore throats. Capillary-dominated flow is modelled based on invasion-percolation rules. Although pore-network modelling is much less resource-demanding than direct simulation approaches, current implementations of the invasion-percolation algorithm are still time-consuming, in particular its phase clustering component, which identifies and determines phase trapping. Computational efficiency is essential when calculation of representative flow properties requires very large pore-network models of 10-100s millions network elements, for example for carbonates that exhibit
multi-scale pore systems, and when performing multiple simulations for uncertainty analysis of, for example, wettability distributions. The present work introduces a new approach, denoted as dynamic phase connectivity, to track the changes in phase clustering after each displacement step. The relative permeability evaluation procedure has been optimised to accommodate for widely accessible multi-core CPU architectures. The combined speed-up factor of the proposed methodology is from two to three orders of magnitude compared to the best conventional pore-network modelling implementations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-H / 450

Dynamical Capillary Network Model Built On Molecular Level Simulation at the Pore Scale

Peter Bryant\textsuperscript{1} ; Ronaldo Giro\textsuperscript{1} ; Rodrigo Neumann\textsuperscript{1} ; Michael Engel\textsuperscript{1} ; Mathias Steiner\textsuperscript{1}

\textsuperscript{1} IBM Research
\textsuperscript{2} IBM Research - Brazil

Corresponding Author(s): rgiro@br.ibm.com

As length scales grow smaller, the behavior of two fluids flowing through a porous media is more and more strongly affected by capillary pressure. The canonical Young-Laplace equation gives a good estimate of the pressure change across fluid interfaces, but it is technically valid only in equilibrium conditions. It is well-known that for two fluids flowing in capillaries, the interfacial pressure change depends on dynamics, such as flow velocity or, more directly, changes to the interface shape. In this work we investigate ways to represent the dynamical state of pore scale flow in a network model that tracks two-fluid interfaces as they move through a series of connected capillaries. The pore scale model consists of molecular level simulations of two fluids flowing through a single cylindrical capillary. The network model consists of a network of cylindrical capillaries of varying lengths and diameters, for which we combine the equations of motion for two fluids with continuity equations to derive a system of differential algebraic equations, which can be solved for the state of the network in time. To link the two simulations, from the pore scale results we extract the dependence of the capillary pressure on flow speed, which can enter in various ways into the equations of motion for the capillary network.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-C / 158

EM heating stimulated water flooding for oil recovery

Grigori Chapiro\textsuperscript{1}

\textsuperscript{1} Universidade Federal de Juiz de Fora

Corresponding Author(s): grigorichapiro@gmail.com

We report a study of heavy oil recovery by combined water flooding and electromagnetic (EM) heating at a frequency of 2.45 GHz used in domestic microwave ovens. A mathematical model describing
this process was developed. Simplified model equations are solved analytically and the solution is presented in an integral form for the one dimensional case. Complete model is solved numerically using Finite Difference Schemes. Experiments consisting of water injection into Bentheimer sandstone cores, either fully water-saturated or containing a model heavy oil, were also conducted, with and without EM heating.

Model prediction was found to be in rather good agreement with an experiments indicating that EM heating induces an overall improvement of the mobility ratio between the displacing water and the displaced heavy oil.

References:


Click here to agree

Poster 1 / 240

Effect of Non-Newtonian Foam on SAG Foam EOR

Rodrigo Salazar Castillo¹ ; Christopher Pönners² ; Sterre ter Haar² ; Martijn Bos¹ ; William Rossen¹

¹ TU Delft
² The University of Texas at Austin

Corresponding Author(s): r.o.salazar@tudelft.nl

Objectives/Scope:
Foam can improve sweep efficiency in gas-injection enhanced oil recovery. Surfactant-alternating-gas (SAG) is a favored method of foam injection due to injectivity and operational considerations. Laboratory data indicate that foam can be non-Newtonian in the high-quality regime, and therefore during gas injection in a SAG process. We investigate the implications of this finding for mobility control and injectivity, by extending fractional-flow theory to gas injection in a non-Newtonian SAG process in radial flow.

Methods, Procedures, Process:
Non-Newtonian behavior in the high-quality regime means the limiting water saturation for foam stability varies as superficial velocity decreases with radial distance from the well. We discretize the domain radially and perform Buckley-Leverett analysis on each ring; solution characteristics are of constant foam quality. For the first time, we show the implications of this behavior for mobility control at the displacement front as well as injectivity. We base the foam-model parameters and the extent of non-Newtonian behavior on laboratory data in the absence of oil. We compare results to mobilities determined by conventional simulation, where grid resolution is limited.

Results, Observations, Conclusions:
For shear-thinning foam, mobility control improves as the foam front propagates from the well, but injectivity declines somewhat with time. The change of mobility ratio at the front can be considerable, given the huge velocity difference between the wellbore and further out. This change is not simply that measured at steady state at fixed foam quality in the laboratory, however, because the foam front in a non-Newtonian SAG process does not propagate at fixed foam quality. Injectivity benefits from the increased mobility of shear-thinning foam near the well. The foam front, which maintains a constant dimensionless velocity for Newtonian foam, decelerates somewhat with time for shear-thinning foam. For shear-thickening foam, mobility control deteriorates as the foam front advances, though injectivity improves somewhat with time. Overall, however, injectivity suffers from reduced foam mobility at high superficial velocity near the well. The foam front accelerates somewhat with time. Overall, injectivity is a complex result of changing saturations and varying superficial velocities very near the well. Conventional simulators cannot adequately represent these effects, or estimate injectivity accurately, in the absence of exceptional grid resolution near the injection well.

Novel/Additive Information:
For the first time we extrapolate laboratory steady-state foam data for non-Newtonian foam to investigate the implications for injectivity and mobility control in gas injection in SAG in the field.
Effect of Salt Dry-out on Shale Gas Reservoir Production Performance

MOHAMMAD JAMSHID-NEZHAD¹ ; Mehdi Zeidouni²

¹ LSU
² Louisiana State University

Corresponding Author(s): jamshidnejad@lsu.edu

Shale gas reservoirs are typically characterized by nanometer pore throats and very low permeability matrix requiring hydraulic fracturing stimulation of horizontal wells. Water is the main fluid used in hydraulic fracturing and a variety of chemicals are mixed with the water each for a different purpose. Given the very low permeability of shales, very high pressure gradients are experienced in order to achieve economic production rates. The pressure drop results in vaporization of the water by the producing gas. The water being vaporized may be the formation water or a mixture of formation water with the stimulation fluids leaked off into the reservoir. The more pressure drop, the more water is vaporized into the gas and, as a result, the more salt dries out. With the nano-meter size pores in shale gas reservoirs and significant pressure gradients required for economic production, the shale gas reservoir permeability can be significantly damaged due to salt deposition. Salt dry-out can significantly reduce the productivity. Significant adverse impact of salt precipitation on well performance were observed in Marcellus shale play where brine salinities are relatively high. In this paper, we model a shale gas reservoir having gas-water thermodynamic equilibrium, and investigate the effects of pressure decline induced by production on salt deposition and its consequences on permeability reduction. Reservoir properties representative of Marcellus shale gas play are considered for this study. Peng-Robinson EOS is used for reservoir fluids (methane and water) modeling. A horizontal well is placed in the middle of the reservoir and hydraulic fracturing is considered to create fractures around the well. Conducting hydraulic fracturing, the fractures are invaded by stimulation fluid. Gas is then produced through the fractures under constant rate constraint and water is allowed to be vaporized. Gas-water flash calculations are performed to evaluate the amount of vaporized water. Water vaporization causes the dissolved salt to be dried-out. Change in porosity and then permeability due to salt dry-out is calculated using Kozeny-Carman formula. Saturation of dried-out salt is evaluated and correlated as a time-dependent skin around the wellbore. The method is verified by modeling salt precipitation during CO₂ injection into an aquifer and comparing the results with 1D analytical solutions found in the literature. Verifying the method, controlling the gas production from shale gas reservoirs by salt dry-out is elucidated.

Effect of Salt Precipitation on Transport Properties of Lacustrine Shale Reservoir: a Case Study from Jianghan Basin, China

Feng Yang¹ ; Boyu Hu¹ ; Yuchen Ma¹

¹ China University of Geosciences, Wuhan
Corresponding Author(s): fengyang@cug.edu.cn

Many lacustrine organic-rich shales formations, deposited in saline basins or the salification stage of freshwater basins, are interbedded with carbonates, sulfates and chlorates minerals. Dissolution and precipitation of salt always happen during extraction of hydrocarbons from lacustrine shale reservoirs. The dissolution of sulfates and chlorates minerals causes reservoir deformation, while the precipitation of salt crystals in confined spaces reduces the permeability of porous network. To data there is no detailed study of the parameters influencing the reduction of pore space by salt crystals and the consequences for transport properties.

In this paper, laboratory experiments were performed to investigate the mechanism of salt precipitation on transport properties of a shale reservoir from Jianghan Basin, China. Static salting-out tests were conducted for univariate analysis of the effect of salt precipitation on petrophysical properties of shale samples. After that, scanning electron microscope was utilized to observe the existence of salt crystals. Dynamic flooding experiments were designed to investigate the effect of salt precipitation, salt particles migration, and effective stress on dynamic permeability of samples. Different scenarios were discussed to link pore clogging with salt damage, and a permeability damage coefficient was proposed to comprehensively characterize the influence of these scenarios on permeability of shales.

Experimental results indicate that porosity and permeability of shale samples can be decreased by 40%-59% and 64%-80% due to salt precipitation, respectively. There are mainly three kinds of salt precipitations: scattered salt particles, salt granulated aggregates, and salt layers. Diameters/thickness of these salt precipitations varies from 1 to a dozen of micrometer. It is shown that pore clogging resulting from salt granulated aggregates is the common problem for damage to flow channel. The damage degree due to salt precipitation is related to the mineral compositions and structure of shales. The proposed permeability damage coefficients of these shales are between 0 to 0.3. Shale samples rich in clay minerals show much more severe permeability reduction than samples rich in sulfates and chlorates minerals. The former is mainly caused by the increased stress sensitive after salt dissolution, while the latter results from salt precipitation. Based on the permeability damage coefficient, an exponential function was developed to model the evolution of permeability as a function of stress sensitive, salt precipitation, and salt particles migration. This study advanced the fundamental understanding about the dynamic damage process of transport properties in lacustrine shale reservoirs.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-B / 801

Effect of Wearing in Impeller Blades of a Denver Flotation Cell on Hydrophobic Silica Flotation at Laboratory Scale

Author(s): Hyunjung Kim¹

Co-author(s): Allan Gomez-Flores ¹ ; Junhyuk You ¹ ; Scott A. Bradford ² ; Graeme W. Heyes ³

¹ Department of Mineral Resources and Energy Engineering, Chonbuk National University
² US Salinity Laboratory, USDA, ARS

Corresponding Author(s): adgfo@bnu.ac.kr

Flotation tests in laboratories are commonly carried out using Denver flotation cells of laboratory size. Since economical and performance impacts due to equipment age can be less obvious at a laboratory-scale than at an industrial-scale, the condition of parts of the cell is overlooked. Maintenance of damaged or old parts might not be carried out. Usually, these parts are not properly replaced after a certain period of use and replaced only when malfunctions occur. Most of the erosion caused by solid particles during the flotation process occurs in the impeller. Therefore, in this study, the effect of wearing of the impeller in a Denver cell on bubble-particle attachment rates was investigated by Computational Fluid Dynamics (CFD) simulations. The focus of the wearing was
in the blades of the impeller. Complete wearing, half wearing, and no wearing are the three different conditions of wearing that were simulated. Simulations of flotation were conducted using a hydrophobized silica of 60, 120, and 240 μm. Operation parameters included an impeller speed of 1200 rpm, a constant air injection of 2 l/min, and a constant bubble size of 1 mm. The preliminary simulation results show that overall bubble-particle attachment rates inside the flotation cell are sensitive to changes according to the impeller wearing, and thus, recoveries can vary according to the damage or erosion in the impeller. Acknowledgements: This research was supported by the Korea Energy and Mineral Resources Engineering Program (KEMREP).

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-D / 685

Effect of capillary induced flow on CO2 residual trapping

Author(s): Maartje Boon

Co-author(s): Hailun Ni; Charlotte Garing; Sally Benson

Stanford University

Corresponding Author(s): mmboon@stanford.edu

One of the main mechanisms to immobilize CO2 during geological carbon sequestration is residual trapping as a result of capillary forces at the pore-scale. It is often assumed that in the capillary dominated regime, capillary equilibrium within the system is reached instantaneously. This approximation is valid for homogeneous systems where the largest scale of heterogeneity is at the pore scale. However, for heterogeneous systems, there is, next to the capillary potential at the pore scale, a capillary potential at the scale of the heterogeneity which will result in capillary induced flow.

We investigate the impact of capillary induced flow on multiphase flow behavior and its implications for residual trapping of CO2 by performing experimental and numerical core-flood tests. The core-flood tests are carried out for a range of sandstone rock cores (including the Fontainebleau, Berea, Bentheimer, and Dundee) containing different heterogeneity features. Observations of the saturation distribution during drainage experiments, obtained with a medical X-ray CT scanner, are used to construct the sub-core scale permeability fields. With the use of the permeability fields and other experimentally obtained multiphase flow properties, the experiments are simulated numerically. The simulations allow us to calculate the capillary potential at the scale of the heterogeneity and to investigate the impact of capillary induced flow on residual trapping.

Our core-flood tests show that capillary equilibration is a function of time and that the time needed to reach equilibrium depends on the scale of the heterogeneity. The results confirm that for relatively homogeneous rocks capillary equilibration occurs almost instantly. For systems with a larger scale of heterogeneity, capillary disequilibrium can exist locally within a core even in the capillary dominated regime. Furthermore, the direction of the heterogeneity (parallel or perpendicular to flow), the scale of the heterogeneity, and the direction of the flow (from low to high permeability or high to low permeability) impact the local capillary forces and, therefore, the capillary pressure and saturation distribution. This can potentially control residual trapping as horizontal low permeability lenses could lead to bypass, while vertical layers could have a big impact on snap-off.

References:
Acceptance of Terms and Conditions:
Click here to agree
**Parallel 10-A / 429**

**Effect of heterogeneity on the mixing of fluids under convective flow**

Juan J. Hidalgo\(^1\); Marco Dentz\(^1\)

\(^1\) IDAEA-CSIC

**Corresponding Author(s):** juanj.hidalgo@idaea.csic.es

Mixing in the presence of convective instabilities in an homogeneous porous media is governed by the behavior of stagnation points where the fluid interface is stretched and compressed. It has been shown that an interface compression model is able to predict the behavior of the scalar dissipation rate. The mixing regimes experienced by these kind of systems are linked to the dependency of compression on diffusion and the interaction between stagnation points and the correlation structure of the velocity field. We apply this approach to an heterogeneous porous media in which the variations in heterogeneity distorts the convection patterns and the way the fluid interface is compressed. We consider a Rayleigh-Bénard instability in which the stagnation points are at a fixed interface and Rayleigh-Taylor instability in which the interface is mobile. Using a stochastic approach we perform a series of numerical simulations using randomly generated conductivity fields realizations with varying statistical properties. Numerical results are used to analyze the impact of variance and spatial correlation of conductivity fields on the way the fluid interface is compressed and on the mixing behavior of the system. The flow structures are visualized by the strain rate and characterized by their correlation length.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 1-D / 837**

**Effect of pore water in rock on cryogenic thermal-shock cracking behaviors**

**Author(s):** Minsu Cha\(^1\)

**Co-author(s):** Caitlin Carter \(^1\)

\(^1\) Texas A&M University

**Corresponding Author(s):** mcma@tamu.edu

Thermally induced cracks can be created when cold fluid contacts a higher-temperature rock. When rock is dry, it first contracts locally near the fluid/rock interface and then fractures in dominantly in tensile mode. However, when rock is saturated or partially saturated with water, the pore water in a rock complicates the behaviors because expanding freezing pore water may interact with mineral skeletons and compete with contracting mineral solids in driving the fracturing. This all occurs in a complex environment of pore and particle structures. When water becomes ice, the volume in increases by 9%, which is larger than thermally-induced shrinkage in geomaterials. Literature regarding freezing saturated porous media investigated slow freezing under low or cyclic thermal gradients occurring in nature. If frozen slowly, water migrates through the porous media by cryogenic suction, leading to ice segregation and lens growth. However, in rapid freezing under extreme thermal gradient using cryogenic fluid, the cryosuction period is postulated to be too brief to allow water migration and the formation of ice lenses because pore water will freeze quickly. This research centers on the effect of pore water on the thermal cracking behavior. The behavior of water-saturated rock under cryogenic temperature was investigated by laboratory experiments. Concrete, sandstones, and shale are prepared as blocks (8"x8"x8") and cylindrical core
specimens (1.5” dia. x 3”). Each specimen type is prepared as dry, partially saturated, and saturated states. Then the specimens are fully submerged in liquid nitrogen. Temperature at the surface of the block is monitored. In microscale (~particle/pore), we investigated how micro fabric is altered/fractured by cryogenic treatment by using SEM and micro-CT. In macroscale (~core/block), we studied macro-scale changes of internal structures caused by the treatment by using micro-CT. In this scale, we also do mechanical testing such as acoustics, permeability, and strength to see effects on macroscale properties.

After the cryogenic treatment of the water-saturated specimens, all major cracks were created near edges during the cryogenic stimulation. In this case, the ice, which is heavily interconnected through pores, was expanding against mineral matrix. Thus, the outer layer of the block exposed to liquid nitrogen experienced water freezing and expanding, whereas the inner block did not. The outer layer expanded laterally, resulting in shear fractures parallel to the exposed surfaces. If cracks were formed from rock contraction (without the effect of ice), more cracks would be located away from and perpendicular to the edges. The block bottom was in direct contact with the cryogen container limiting liquid nitrogen access resulting in the absence of cracks there. We also present micro CT and scanning electron microscopy results, which reveals interesting interaction between expanding ice crystals and mineral skeletons at specimen surfaces as well as internally.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-F / 342

Effect of retention sites toward silver nanoparticles immobilization in porous media

Author(s): Veronica Morales¹

Co-author(s): Janis Patino ¹

¹ UC Davis

Corresponding Author(s): janpatino@udavis.edu

Column tests are a widely used experimental tool to investigate particle transport in porous media. However, different experiments can produce similar breakthrough curves, which make these data insufficient in order to understand the governing processes that control particle transport under different conditions. Profile analysis of the deposited particles provides information about the particle distribution in the packed column, but this method involves the destruction of the column and it is subject to many uncertainties during the sample extraction. A novel non-invasive technique, based on x-ray tomography, is proposed for the study of silver nanoparticles (n-Ag) distribution in uniform porous media (glass bead packed column) under both saturated and unsaturated conditions.

Column experiments were performed using a model porous medium of glass beads through which colloidal silver particles were transported under conditions of varying water content. X-ray microtomography was subsequently employed as a non-destructive imaging technique to obtain information on i) the presence and distribution of the different retention sites contributing toward particle immobilization, ii) retention-site specific profiles of immobilized colloids, iii) morphological characteristics of the deposited colloidal aggregates, and iv) channel widths of pore-water network representations.

Therefore, we provide a statistical evaluation of the significance of colloid retention by attachment to the liquid-solid, gas-liquid, gas-solid interfaces, and by straining. Additionally, an effective-pore structure characteristic is proposed to improve predictions of mass removal by straining under various water saturations. The novel procedure leads to the understanding of the pore-scale sites that are responsible for particle retention and their specific contribution to the total filtration process, also allowing revision and strengthening of the mechanistic models describing fate and transport of particles in porous media.
Parallel 8-A / 538

Effect of salinity on the transport of heavy metals and radionuclides in reactive porous media

Zi Ye\textsuperscript{None}, Valentina Prigio\textsuperscript{bNone}

Corresponding Author(s): zye4@stevens.edu

Hydraulic fracturing (or fracking) is a well stimulation technique for unconventional oil and gas extraction\textsuperscript{1}. Around 8-38 million cubic meters of fracking fluid containing water, chemicals, and sand are injected into the shale every day [2]. High-pressure injection of fracturing fluids allows to create fractures and mobilize the gas and the oil towards the surface. Together with the gas, a hypersaline brine (i.e., the flowback and the produced water) is extracted which contains heavy metals and radionuclides, such as barium, strontium, and radium. Spills of flowback and produced water into the subsurface may occur during operation, handling, and storage with potential negative impact on potable aquifers. However, the behavior of the heavy metals and radionuclides at the condition of hypersaline brine has not been studied, yet.

Here, we present an experimental and modeling work to describe the effect of salinity on the transport of the major cations in the produced water. We selected goethite-coated silica beads as reactive material. We performed column-flood experiments using both produced water (obtained from MSEEL, WV) and synthesized produced water. A triple layer model (TLM) [3] was developed and implemented in PHREEQC to simulate the metal transport behavior. Preliminary experiments were performed by injecting a pH 8 solution containing barium at various salinity into a column filled with goethite-coated beads. Results show that the retardation of barium significantly decreases with salinity due to its decreasing free ion activities. This suggests that in a case of a spill of produced water within an aquifer containing iron-oxide mineral, a fast migration of the major cations may occur with a potential negative impact on aquifer water quality.

References:


Parallel 5-G / 964

Effect of select naphthenic acids on oil-water interfacial dynamics

Teresa Reilly\textsuperscript{1} ; Teresa Lehmann\textsuperscript{1} ; Vladimir Alvarado\textsuperscript{1}

\textsuperscript{1} University of Wyoming

Corresponding Author(s): treilly2@uwyo.edu

Injection of a generic naphthenic acid blend to injection brine has been shown to increase oil recovery. The purpose of this work is to analyze the effect of several individual naphthenic acids
on the oil-water interfacial dynamics. Acids were selected based on water solubility and structure; analysis of different structural characteristics of various acid groups was made to determine a possible connection of the interfacial response with respect to molecular structure. Oil-brine Interfacial visco-elasticity data were collected for the select acids using an AR-G2 rheometer with the double-wall ring geometry. High-field Nuclear Magnetic Resonance (NMR) and pH measurements were taken on the aqueous phase of the rheology experiments to quantify acid concentration. Low-field NMR droplet size distribution measurements were conducted on water-in-oil emulsions prepared with different acids. High-field NMR data show that added acids tended to partition into the oil phase or to the interface at the end of the five-day experiments. pH is measured for both the before and after instances and was found to correlate with NMR observations. Generally, acids lower the visco-elasticity compared to the un-acidified brine; acids with similar structures induce similar dynamic interfacial responses. High visco-elasticity values have been shown to increase connectivity of the oil phase in microfluidic devices in past experiment. Low-field NMR droplet size distribution measurements indicate that acids in bulk destabilize emulsions, while most individual acids examined show an increase in stability, compared to the low-salinity brine in which they are solubilized. Emulsion stability data also show a dependence on acid structure. Data show that even small concentrations of individual naphthenic acids affect the visco-elasticity and the stability of emulsions. Based on the fluid-fluid interactions examined, the effective core-flood acid blend contained several of the acids examined in this work.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-G / 34

Effective Models of Flow in Vuggy Carbonate Reservoirs

Mojdeh Rasoulzadeh¹ ; Fikri Kuchuk²

¹ University of Alabama
² Schlumberger

Corresponding Author(s): mrasoulzadeh@ua.edu

Carbonate reservoirs hold almost half of the world’s oil and gas reserves. Many giants carbonate fields are rather mature, been producing for 50 or even 100 years; these are ready for some form of gas-flooding, EOR. More precise reservoir characterization can lead to better modeling of EOR schemes for these giant/mature fields. Characterization of carbonate reservoirs is a complicated task mainly because of the complex texture and pore network. Heterogeneities are present in all the scales as well as anisotropy in vertical and horizontal directions. The presence of vugs and fractures in carbonate rock can significantly affect pressure and flow behavior of the fluid. A vug is a cavity (usually a void space, occasionally filled with sediments), and its pore volume is much larger than the intergranular pore volume. Current laboratory techniques may not be capable of quantifying the vuggy heterogeneities in carbonate reservoirs and interpret the effect of the presence of vugs on the permeability of porous media.

This is mainly because of the practical limits of core samples preparation and the variety in size of heterogeneities in carbonate rock. The vug size can be larger than core samples, and consequently, no lab technique can capture the effect of vug on the petrophysical parameters of the carbonate rock. The core sample analysis usually underestimates the carbonate rock’s permeability.

We use the analytical models for flow in heterogeneous porous media, including a random distribution of fluid-filled vugs and karsted zones (we address them all as the vuggy inclusions). The flow in vugs at the microscopic level does not obey Darcy’s law; rather it is governed by Stokes flow. The coupling of Stokes flow and Darcy’s law is implemented through a no-jump condition on normal velocities, a jump condition on pressures, and generalized Beavers–Joseph–Saffman condition on the interface of the porous matrix and vug or fracture. The spheroidal geometry is used because of its flexibility to represent many different geometrical shapes. A spheroid reduces to a sphere when the
focal length of the spheroid approaches zero. A prolate spheroid degenerates to an elongated rod to represent the connected vug geometry (a tunnel geometry) when the focal length of the spheroid approaches infinity. An oblate spheroid degenerates to a flat spheroidal disk to represent the fracture geometry. The effective permeability of a porous medium including random distribution and size of vugs as well as a binary porous medium with a uniform distribution of vugs is obtained.

References:
Yao J. Huang ZQ. Fractured Vuggy Carbonate Reservoir Simulation; 2016 Jul 28, Springer. Acceptance of Terms and Conditions:

Click here to agree

Parallel 6-H / 6

Effective elastic properties of porous media and metamaterials

Willi Pabst¹ ; Eva Gregorová¹ ; Tereza Uhliřová²

¹ University of Chemistry and Technology, Prague
² UCT Prague

Corresponding Author(s): pabstw@vscht.cz

Porous media can be viewed as a special type of two-phase composites (with one phase being the void phase or possibly vacuum) or as metamaterials (i.e. materials with microstructures that are principally similar to macroscopic architectural structures, from which they differ only by scale) [1,2]. In this contribution we investigate the effective elastic constants of isotropic and cubic porous media or metamaterials. The computer-generated digital microstructures studied include convex pores (spherical, spheroidal-oblate, spheroidal-prolate), concave pores (i.e. intergranular voids between spherical or spheroidal grains), and foams (strut-based or wall-based Kelvin or random foams with open or closed cells). Numerical calculations are used to obtain the effective constants (stiffness matrix) of these model microstructures. The results are compared to the micromechanical bounds (upper Wiener-Paul and upper Hashin-Shtrikman bounds) and to the admissible predictive model relations (i.e. power-law relations and our exponential relations [3-5]; other model relations occurring in the literature are shown to be either redundant or wrong, and it is shown that so-called minimum solid area model are useless for the prediction of effective elastic properties of materials with concave pores [6]). While the power-law and exponential relations provide tentative predictions that are more or less realistic for the effective elastic properties of materials with convex pores and foams, they are seriously in error for materials with concave pores, grossly overestimating the true values. In order to circumvent the (highly nontrivial) problem of quantifying a large number of microstructural descriptors and the (so far unsolved) problem of implementing this microstructural information into microstructure-property relations, cross-property relations between the elastic moduli and thermal conductivity can be used. In particular, it is shown that our cross-property relation for spherical pores [7] provides excellent predictions of the tensile modulus (Young’s modulus) and shear modulus in all cases of isometric pores, spherical or not, including the case of concave pores, which cannot be predicted by any analytical model relation. Moreover it is shown that our recently proposed generalized cross-property relation for spheroidal pores [8] can predict the elastic properties even in the case of randomly oriented anisometric (spheroidal) pores.
References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-F / 990

Effects of Bacterial EPS on Drying of Porous Media

Wenjuan Zheng¹ ; Saiqi Zeng¹ ; Jacob LaManna² ; Harsh Bais¹ ; Yan Jin¹

¹ University of Delaware
² National Institute of Standards and Technology

Corresponding Author(s): wendyzh@udel.edu

Drying of porous media is of significant importance in many fields ranging from hydrology and agriculture, to industrial applications, e.g., food sciences and chemical engineering. The drying process depends on both the external atmospheric conditions and structure of the porous medium. Previous research has shown that hydrogel produced by plant seeds/roots or bacteria can change the physical and hydraulic characteristics of porous media, however, the role of hydrogel on the drying process remains unclear. In this study, we measured water evaporation in Accusand (40/50 mesh) as influenced by bacterial EPS (extracellular polymeric substances; produced by Bacillus subtilis strain FB17) and a bacterial EPS surrogate xanthan using weight measurements and neutron radiography imaging (NRI). Less evaporative water loss, slower Stage I evaporation, and shorter duration of Stage I evaporation were observed for EPS-amended samples than their corresponding controls. We discussed three mechanisms that are potentially responsible for the observed EPS effects, (1) large water holding capacity of EPS, (2) broader effective pore size distribution, and (3) modification in physicochemical properties (reduced surface tension and increased viscosity) due to EPS presence. These findings improve our understanding of the drying process as affected by hydrogel, with the potential application in engineering rhizosphere for agriculture production under restricted water availability.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 5-E / 531

Effects of Confinement and Surface Force on Methane Hydrate in Porous Media

Author(s): Dongliang Jin

Co-author(s): Benoit Cosane

1 CNRS and Laboratoire Interdisciplinaire de Physique (LIPHY), Universite Grenoble Alpes, F-38000 Grenoble, France
2 CNRS/University Grenoble Alpes

Corresponding Author(s): dongliang.jin@univ-grenoble-alpes.fr

Methane hydrate is a non-stoichiometric crystalline structure in which water molecules form hydrogen-bonded cages with methane molecules inside. Abundant methane hydrate resources are present on Earth, especially in various mineral porous media (e.g., clays, coal, shale, permafrost and sea-floor). Understanding the dynamics and thermodynamics of methane hydrate confined in porous media has therefore attracted a great deal of attention in the last decade.

In the present work, we combine computer modeling and theoretical approaches to determine the dynamics and thermodynamics of methane hydrate confined in porous media. First, molecular simulation, including Molecular Dynamics (MD), Monte Carlo simulations (using direct coexistence method), and free energy calculations (involving Einstein Molecule approach and umbrella sampling), is used to show that the shift in melting temperature of methane hydrate confined in porous media with respect to the bulk phase at a given pressure, \( \Delta T_m = T_{m}^{\text{pore}} - T_{m}^{\text{bulk}} \), is negative. Then, the surface tension of methane hydrate \( \gamma_{HS} \) and liquid water \( \gamma_{WS} \) in porous media is determined to rationalize these results. We also demonstrate that the pore size \( (D_p) \) effect on \( \Delta T_m \) can be well predicted by the Gibbs-Thompson equation, \( \Delta T_m/T_{m}^{\text{bulk}} \sim 1/D_p \), with \( \gamma_{HS} < \gamma_{WS} \). Finally, isobaric-isothermal and canonical ensemble MD simulations are used to determine several important thermodynamic properties of methane hydrate confined in porous media: (a) the thermal conductivity \( k \) is evaluated by Green-Kubo integral of the autocorrelation function of the heat-flux vector (JACF); and (b) the thermal expansion \( \alpha_P \) and isothermal compressibility \( k_T \) are determined according to their definitions: \( \alpha_P = \frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T \) and \( k_T = -\frac{1}{V} \left( \frac{\partial^2 V}{\partial T^2} \right)_P \). Comparison with data for bulk methane hydrate and experimental results will be made.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-A / 527

Effects of Groundwater Circulation Well to contaminant Back-Diffusion from low-permeability layers: investigation by laboratory test and numerical simulations.

Fabio Tatti, Marco Petrangelii Papini, Paolo Viotti

1 Department of Civil, Building and Environmental Engineering (DICEA), University of Rome "La Sapienza", Rome, Italy
2 Department of Chemistry, University of Rome "La Sapienza", Rome, Italy

Corresponding Author(s): fabio.tatti@uniroma1.it

The presence of contaminants in low permeability zones of aquifer can represent a real limitation for a complete and effective groundwater restoration. When dissolved plume encounter low permeability layers, concentration gradient between low and high-permeability zones determines storage of dissolved pollutants into the lower permeability layers by molecular diffusion (Forward-Diffusion).
After the end of the plume passage there is an inversion of the gradient direction that leads to a slow re-distribution of contaminant from the lower permeability zones back to the higher permeability zones (Back-Diffusion). The low-permeability zones become therefore secondary contamination sources that cause long plume tail.

The aim of this study was to evaluate by laboratory test and by numerical simulations the suitability of Groundwater Circulation Well (GCW) to restore contaminated low permeability zones of aquifer. GCW is a well characterized by a different number of screens with extraction induced from one screen and injection from another. The use of GCW develops a circulating flow field near the well, increasing the vertical component of groundwater flow.

A sand aquifer with two low-permeability lenses was reconstructed inside a tank containing a GCW model. The lenses were saturated with a known quantity of tracer and a circulating flow field was generated inside the aquifer injecting clean water from the upper GCW screen and extracting contaminated water from the lower screen. During the test, images of the box model were acquired and using an image analysis procedure the tracer mass released by the two lenses was estimated.

A numerical model was developed to reproduce the Back-Diffusion process and to investigate effects of pumping technologies to contaminant redistribution process from low to high permeability zones of aquifer. The model was validated comparing the numerical results with those obtained experimentally by laboratory test. Numerical simulations were carried out to evaluate effects of innovative GCW technology and traditional Pump and Treat system on the Back-Diffusion process. To achieve the goal, numerical tests were performed considering various injection/extraction water flow rates and different features of polluted low permeability layers.

Results demonstrate the more suitability of the GCW technology to restore contaminated low permeability zones than the traditional Pump and Treat system. However, the efficiency of GCW appear to depend on features of low-permeability layers, as their geometry and their position inside the aquifer.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-G / 980

Effects of Shapes of Pore Throat on Water Infiltration under Microgravity.

Author(s): Natsumi Naganuma

Co-author(s): Naoto Sato ; Yuichi Maruo ; Kent Nogawa ; Kosuke Noborio

1 Graduate School of Agriculture, Meiji University
2 Meiji University

Corresponding Author(s): n.n.rsh.0414@gmail.com

Crop production using soil on Moon or Mars will be needed for a long-duration space mission. Water movement in porous media under microgravity must be known for agriculture in space. Water in porous media is mainly moved by a matric potential gradient. According to previous research, water movement in soil is extremely slower under microgravity than under 1G although a capillary force, which is the main contributor to matric potential, is apparent in microgravity. We conducted drop-tower experiments to reveal why the infiltration rate of water in porous media became slower under microgravity conditions. We hypothesized that specific pore shapes among soil particles and changes in the contact angle between water and soil particles made water move slower in porous media under microgravity. Various capillary shapes were made with acrylic and polycarbonate materials to carry out capillary rise experiments using distilled water and various concentrations of aqueous ethanol solutions (10, 40, 75, and 100% v/v). Droplets of distilled water were made on acrylic and polycarbonate plates to measure contact angles under both microgravity and 1G conditions. We found that capillary shapes affected a water rise rate whereas the contact angles of droplets with small capillary length hardly changed.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-A / 66

Effects of Wettability and Permeability on Viscous Fingering during Unstable Immiscible Displacements

Bochao Zhao \^; Kishore Mohanty \(^1\)

\(^1\) The University of Texas at Austin

Corresponding Author(s): bchao.zhao@gmail.com

During water flooding of viscous oil reservoirs, adverse mobility ratio leads to an unstable displacement and thus viscous fingering. Previous research in viscous fingering has focused on low flow rates and high permeability systems (above 1 Darcy). This paper provides a more thorough and systematic study of the factors affecting viscous fingering including lower permeability, different wettability and high flow rate. Homogeneous cores with permeability ranging from 20 md to 6 Darcy are selected for unstable coreflood experiments. For water-wet systems, water is used to displace viscous mineral oil of different viscosity. For weakly oil-wet (mixed-wet) systems, the core is aged in a crude oil and water displaces a viscous oil. To study strongly oil-wet system, the fluid phases are switched. A light hydrocarbon is used to displace a viscous water in a water-wet core, which is invasion of a strongly non-wetting fluid (similar to water invasion in an oil-wet rock). The effects of permeability, wettability and flow rate on fingering and oil recovery are studied. Unstable displacements are also conducted in micromodels to allow easy visualization of pore-scale mechanisms.

For water-wet systems, decreasing permeability leads to more intense fingering and lower recovery. Increasing flow rate leads to consistently lower recovery due to less time for the imbibition of water into oil-filled pores. \(N_{vf} = N_e (\mu r^2) / (D^2)\) can be used to correlate recovery in the presence of viscous finger for water-wet systems. Weakly oil-wet (mixed-wet) systems show distinctively different flow patterns than strongly oil-wet and water-wet systems. For strongly oil-wet systems, permeability does not have a significant effect on fingering and recovery. At low flow rates, increasing flow rate leads to a higher recovery because the higher pressure in the finger can overcome the capillary pressure and invade oil-filled pores. However, further increase in flow rate enhances fingering and results in lower recovery. There exists an optimum flow rate to yield the highest recovery in strongly oil-wet systems. \(N_{vs} = [N_{e} (r^{-1}) / \mu r^2 D^2] = 2\) can be used to correlate recovery in the presence of viscous finger for strongly oil-wet system. Viscous fingering is more intense in oil-wet systems than in water-wet systems. Water film flow in water-wet systems damps viscous fingering, but there is little oil film flow in strongly oil-wet systems due to the high oil viscosity.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 593

Effects of wettability on two-phase relative permeability estimates from direct pore-scale simulations

Author(s): Gaël Raymond Guédon \(^1\)

Co-author(s): Paolo Lurati \(^2\); Fabio Inzoli \(^1\); Monica Riva \(^2\); Alberto Guadagnini \(^2\)

\(^1\) Politecnico di Milano, Dipartimento di Energia

\(^2\) Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
Corresponding Author(s): gaelraymond.guedon@polimi.it

We present a numerical analysis of fluid phase distributions and relative permeabilities obtained from direct pore-scale simulations of two-phase flow through a real pore space with diverse conditions of wettability. Exploring the effects of wettability on the fluid behaviors within porous media is of fundamental relevance for a variety of engineering as well as environmental applications, including, e.g., conventional and unconventional hydrocarbon extraction, along with CO2 storage in subsurface systems. The pore space investigated is a three-dimensional limestone rock reconstructed via X-ray micro-tomography at 2 microns voxel size resolution. The one millimeter-scale rock sample is associated to a connected porosity Phi = 0.128 and an absolute permeability k = 357 mD. We employ a simulation procedure mimicking steady-state protocols implemented to estimate multiphase relative permeability by laboratory-scale experiments. We first simulate a primary-drainage (oil injection) process until steady-state conditions are reached. Then, we simulate a series of secondary-imbibition (water injection) processes by injecting diverse amount of water/oil volumes until steady-state conditions are achieved. The ratios between oil and water densities and viscosities are set equal to 0.78 and 2.87, respectively. In all our simulations the capillary number is constant and equal to 1 to 5. Flow field and fluid phase distributions are calculated within the explicit three-dimensional pore space using a finite volume-based solver and implementing the so-called Volume-Of-Fluid technique. Capillary end effects that may arise at the inlet and outlet boundaries are removed by implementing ad-hoc periodic conditions (see ref [1]). In this context, adjustment of fluid-phase saturations is achieved through local injection of one of the two fluids. The total fluid flow rate is indirectly set through a pressure jump across the periodic inlet and outlet boundaries. Simulations were achieved using HPC resources at CINECA computing center [2], within the LISA-Prod Project HPL13P71U0. In order to assess the impact of wettability conditions on the resulting two-phase relative permeability curves, multiphase flow simulations are performed by using diverse contact angle values at the solid-fluid boundaries resulting in water-, neutral- and oil-wet conditions. The numerical errors associated with both geometry and pore space discretization are analyzed by performing a sensitivity analysis reconstructing the pore-space with diverse spatial resolution scales. We observe that errors in the geometrical representation have an impact on the averaged capillary pressure as well as on residual fluid saturations, while errors originating from the pore-space discretization impact water and oil relative permeabilities. Our results document that varying the contact angle has a strong influence on residual oil and water saturations, relative permeability curves and spatial distribution of fluid phases observed at the end of the primary-drainage and secondary-imbibition processes.

References:


Click here to agree

Poster 2 / 471

Efficient Nonlinear Gauss-Seidel Type Solvers for Black-Oil Type Models

Oystein Klemetsdal¹; Olav Møyner²; Atgeirr Rasmussen³; Knut-Andreas Lie³

¹ NTNU
² SINTEF, NTNU
³ SINTEF Digital

Corresponding Author(s): oystein.klemetsdal@gmail.com

Models for multiphase flow in porous media account for several complex physical phenomena such as PVT behavior and interplay with the porous rock, which altogether make reservoir simulation a challenging task. High aspect ratios and strong petrophysical heterogeneity impose severe timestep (CFL) restrictions, and implicit discretizations are thus usually preferred over explicit ones. In a fully
implicit discretization, one must solve a large nonlinear system of equations to advance the solution in time. In many cases, the computational cost can be significantly reduced by splitting the overall equation system into a pressure equation and one or more transport equations, and solve the two subproblems sequentially using specialized solvers.

Herein, we consider how to solve the transport equations as efficient as possible. For cases without capillary forces and with co-current flow only, the unknowns within a given cell will only depend on unknowns in the cell’s upstream neighbors. By sorting the cells based on the total inter-cell fluxes, the flow equations can thus be permuted to a triangular form and solved very efficiently in $O(n)$ in a cell-by-cell fashion. In the general case, the reordered system will also contain diagonal blocks consisting of multiple cells that are mutually dependent. These larger blocks can either be solved using a standard Newton-Raphson method or by a Gauss-Seidel method that sweeps repeatedly through the cells in some predefined order.

In this talk, we demonstrate the applicability of the reordering method to realistic reservoir configurations, and show how we can use the sequential splitting with reordering either as a standalone solver, or as a nonlinear preconditioner for the fully implicit nonlinear system.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-C / 658

Efficient VOF simulations of pore-scale multiphase flow

Stéphane Zaleski1

1 Institut Jean Le Rond d’Alembert

Corresponding Author(s): stephane.zaleski@gmail.com

We describe recent advances in pore scale dynamics direct numerical simulation. The Volume of Fluid method associated with well-balanced surface tension methods allows for the simulation of low capillary numbers. Further progress should involve thin film and corner flow formation, contact line dynamics and efficient combinations of parallelism and grid adaptation.

This ensemble of approaches is expected to particularly interesting for enhanced oil recovery modelling.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 796

Efficient liquid transport induced by drying paste/substrate systems

Mohamed Nidal BEN ABDELOUAHAB1 ; Alban Gossard2 ; Stéphane Rodts3 ; Philippe Coussot3

1 CEA Marcoule - Laboratoire Navier
2 CEA Marcoule
3 Univ. Paris-Est
**Corresponding Author(s):** mohamednidal.benabelouahab@cea.fr

Poilutice technology is currently mainly used for the desalination of masonry structures in the field of architectural heritage conservation. Wet poilutices are coated on the porous material to be treated, and kept in place before being removed when dry. The efficiency of the process basically depends on the drying behavior of the system poilutice/substrate, but so far little is known concerning drying of systems composed by soft materials applied to substrate surface. Here we show that, in contrast with various other materials (polymers, smectite clay, silica gel, latex, cellulose, etc) kaolin clay pastes have unique absorption properties as they may extract almost all the liquid (and the suspended elements) from the porous medium at a high rate.

We followed drying of different poilutice systems coated on a substrate (glass microbeads with two different pore size), with Nuclear Magnetic Resonance (NMR). Different NMR sequences were used which provided the evolution of key internal characteristics in time: 1) the water saturation distribution; 2) transverse and longitudinal relaxation spectrum; 3) the poilutice shape (shrinkage). From this information we identified the different drying regimes of poilutice/substrate systems in relation with their microstructure evolution.

The remarkable properties of kaolin pastes appear as follow. In a first period, the paste shrinks axially (along the direction of evaporation) without fracturing, so that it maintains a full coverage of the porous medium surface. At the end of this period the material has formed a solid porous structure which, interestingly, will resist capillary pressure during the next steps of the process. When the pore size of this system is smaller than that of the substrate the liquid is progressively extracted from the substrate, while the poilutice apparently remains (on average) saturated. In fact, air necessarily penetrates the kaolin paste in the form of transient paths reaching the substrate then closing back. This period lasts until almost 90% of water initially in the substrate is evaporated. A third period starts once capillary forces inside the poilutice and the substrate are balanced. The water saturation now decreases almost homogeneously throughout poilutice and substrate. Surprisingly, despite these complex processes, the drying rate in both the first and second period remains constant (i.e. at its initial, possibly high, level). This implies that almost all the water contained in substrate moves through the poilutice to be evaporated at its free surface under approximately constant conditions [2]. This also implies that in general the elements suspended in the liquid will be transported and finally accumulated inside the poilutice, which means that such a material is remarkably efficient.

**References:**


**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 1-E / 582**

**Efficient molecular simulations of binary gas mixture transport in slit nanopores**

**Author(s):** Tianhao Wu

**Co-author(s):** Abbas Firoozabadi

---

1 *Reservoir Engineering Research Institute (RERI)*

**Corresponding Author(s):** tianhaowu.pku@gmail.com

A novel approach is suggested to simulate the gas mixture transport in slit nanopores. The proposed method is based on the modification of the dual control volume grand canonical molecular dynamics (DCV-GCMD) method. The conventional method, DCV-GCMD, describes the gas mixture transport...
with pre-set constant composition. Due to the selective adsorption in the nanopores, the composition of the produced gas mixture will be affected. The modified method provides the composition in the permeate side. Gas mixtures of CH4/He and CO2/CH4 are investigated in graphene, graphite, and clay slit nanopores. The results show that pore size is the dominant factor in the species separation; the solid surface roughness has pronounced effect on gas separation; the influence of average pressure is not pronounced. The effects of pore length, temperature, pressure gradient, and feed composition are also investigated.

References:

Acceptance of Terms and Conditions:

Click here to agree

1126

Electrokinetic Transport at Micro/Nanoscale Coupled with Surface Chemistry

Moran Wang1; Li Zhang2

1 Tsinghua University Department of Engineering Mechanics
2 Tsinghua University

Corresponding Author(s): mrwang@tsinghua.edu.cn

Surface charge at solid-electrolyte interface is generally affected by the local physical and chemical properties in the solution such as ionic strength, pH and so on. In a system with concentration or pH variation, rather than the prevailing assumption of homogeneous surface change, it leads to a spontaneous inhomogeneous distribution of surface charge, which has been observed in geotechnical engineering, membrane science and microfluidics, but never been well understood. Further complexity comes from the multiscale feature of the electrical double layer (EDL) and its overlapping at micro/nano scale. Here, to tackle this coupled electrokinetic transport process, we present a general modeling strategy based on a classification using the ratio of the Debye length to the characteristic pore size. We show that this classification can be applied in modeling electro-osmosis (EOF) from a thin EDL to a fully overlapped EDL. The effect of inhomogeneous surface charge on electrokinetic velocity and permeability is discussed. This effect plays an important role in observed phenomena such as flow reversal in electrokinetic remediation and electro-osmotic hysteresis in EOF displacement.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-A / 787

Electrokinetic Transport at Micro/Nanoscale Coupled with Surface Chemistry
Moran Wang1; Li Zhang2

1 Tsinghua University Department of Engineering Mechanics
2 Tsinghua University

Corresponding Author(s): mrwang@tsinghua.edu.cn

Surface charge at solid-electrolyte interface is generally affected by the local physical and chemical properties in the solution such as ionic strength, pH and so on. In a system with concentration or pH variation, rather than the prevailing assumption of homogeneous surface charge, it leads to a spontaneous inhomogeneous distribution of surface charge, which has been observed in geotechnical engineering, membrane science and microfluidics, but never been well understood. Further complexity comes from the multiscale feature of the electrical double layer (EDL) and its overlapping at micro/nano scale. Here, to tackle this coupled electrokinetic transport process, we present a general modeling strategy based on a classification using the ratio of the Debye length to the characteristic pore size. We show that this classification can be applied in modeling electro-osmosis (EOF) from a thin EDL to a fully overlapped EDL. The effect of inhomogeneous surface charge on electrokinetic velocity and permeability is discussed. This effect plays an important role in observed phenomena such as flow reversal in electroketic remediation and electro-osmotic hysteresis in EOF displacement.

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 981

Electrophoresis to improve cement-steel bonding in well construction

Alexandre Lavrov1; Ragnhild Skorpa1; Malin Torsater1

1 SINTEF

Corresponding Author(s): malin.torsater@sintef.no

After production, all wells need to be permanently plugged and abandoned (P&A’ed). Long-term well integrity will then rely on the integrity of cement, which is the material typically used for permanent well plugging and for filling the annular spaces between casing/rock. The cement is pumped into the well as a slurry, and hardens to form mechanical and hydraulic seals. Cement has proven to be a robust material for subsurface constructions, but concerns are directed towards the interfaces between cement/rock and cement/casing. These are prone to delamination (commonly referred to as “debonding”) and can thus act as leakage paths for formation fluids (oil, water, gas) along the well. In order to reduce the long-term environmental impact of oil and gas production activities, it is thus necessary to improve this “weak link” of today’s well construction.

Bonding between cement and steel is controlled by the material structure and packing in the interfacial transition zone (ITZ), a thin (50-100 micron wide) zone located in cement near the steel surface. Applying positive potential on the steel wall improves the bonding and thus could be used to improve long-term well integrity in the field. In downhole conditions, however, cements are subject to
elevated pressure and temperature. Moreover, composition of well cements is usually designed so as to stabilize the slurry and thus to reduce attractive forces between the particles. These operational factors may adversely affect the efficiency of such electrophoresis-induced bonding enhancement. Experiments are performed in order to investigate the effect of different operational factors (ionic strength, zeta-potential, particle size distribution, additives in cement) on the electrophoresis-induced bonding enhancement. A mesoscopic particle-based model is constructed and used to study the effect of operational factors on the process. The model is based on the discrete-element method (DEM) where particle interactions are introduced via the lubrication force. The lubrication accounts for, in general, non-Newtonian rheology of the carrier fluid in the cement slurry. Stokes flow is assumed. The model enables two-way coupling between the electric field and the particles. It also accounts for the effect of electrolysis near anode upon the particles.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-D / 781

Enhanced grain partitioning of microtomography segmented images

Nicholas Skrivanos1 ; Karsten ThompsonVone

1 Louisiana State University Petroleum Engineering Department

Corresponding Author(s): nskriv2@lsu.edu

Grain partitioning of three-dimensional microtomography segmented images provides valuable in-situ property and structure characteristics of porous media samples. There are many applications of this technology, ranging from analyzing core samples in petroleum engineering and soil science to developing novel structures in material science. This information can be further used as a tool to generate more accurate particle packings for simulations, and also as a base for geo-mechanical models. The overall objective of this work is to improve the accuracy and reliability of grain-partitioning algorithms applied to microtomography or other three-dimensional images.

The methodology described here is broken into two separate categories: initial partitioning, and post processing refinement. The initial partitioning is based upon a Euclidean distance map of the sample and the watershed algorithm, meaning that this methodology assumes that the particle interfaces coincide with watershed surfaces. In order to combat the over-partitioning that is common with this methodology, several new iterative techniques have been implemented into particle assembly. Once the initial partitioning is completed, the user has the opportunity to interact with the resulting image and to directly apply refinement options such as planar regression for particle contacts, automatically merging particle pairs meeting a specified criteria, and manually merging individual particular pairs. Bulk and individual properties, such as porosity, particle volumes, surface areas, contact areas, and aspect ratios are calculated and updated corresponding to any refinement.

More advanced analysis through machine learning is also being investigated. After the initial partitioning, the user is shown pairs of grains, as well as their neighbors, and is prompted to make a decision on whether or not the subject grain should be merged together. All statistics regarding the grains of interest are recorded along with the user’s decision. After a sufficient number of decisions have been recorded for the given sample, logistic regression is performed on the recorded data, and compared with the cross validation data. Once a specified accuracy is met, the resulting logistic regression equation can be applied to the remaining portions of the porous media sample, and other images with similar particle and structural characterization.

References:

Acceptance of Terms and Conditions:
Enhanced pH-dependent transport in porous media

Ting Liu\textsuperscript{1}, Marc Hesse\textsuperscript{1}, Valentina Prigio\textsuperscript{1}

\textsuperscript{1} The University of Texas at Austin
\textsuperscript{2} Stevens Institute of Technology

Corresponding Author(s): tlui18@stevens.edu

When a solvent carries cations through a soil with fixed capacity for adsorption or ion exchange, the evolution of concentration fronts, which propagate through the soil at characteristic fractions of the solvent flow speed, is well described by classical theory. When the soil contains hydrophilic minerals such as iron oxyhydroxide, quartz, and clays which readily adsorb and desorb protons, and when the pH of solvent differs from the pH of the soil, non-classical concentration fronts can arise, in addition to the classical. We will present experimental results and theoretical solution compared with numerical simulations.

A manifestation of classical pH-dependent transport occurs when low pH solvent (e.g., brine saturated with CO\textsubscript{2}) enters a soil containing adsorbed cations. The acidified brine favors the formation of a desorbing front moving slower than the flow speed, but characterized by a peak whose maximum concentration, controlled by the brine pH, can be much larger than the initial value presenting a health hazard.

The manifestation of non-classical behavior is the anomalously rapid solute transport that occurs when a solvent at high pH enters a low pH hydrophilic mineral-bearing soil. In addition to a classical retarded front, a non-classical pulse forms which travels at the flow speed much faster than expected. It is due to the combination of hydrodynamic dispersion and pH-dependent adsorption. Dispersion creates a low pH mixing zone within the initial front where cation adsorption is negligible; it detaches from the retarded front and travels un-retarded ahead of it.

References:

Acceptance of Terms and Conditions:
Click here to agree

Enriched Galerkin approach for density-driven flow in unsaturated coastal aquifer

Author(s): Jonghyun Lee\textsuperscript{1}

Co-author(s): Sanghyun Lee \textsuperscript{2}

\textsuperscript{1} University of Hawaii at Manoa
\textsuperscript{2} Department of Mathematics, Florida State University

Corresponding Author(s): jonghyun.harry.lee@hawaii.edu

Accurate numerical simulations for density-dependent flow and transport model is one of the crucial keys for successful water resources management in coastal areas and on islands. However, traditional modeling approaches without special treatment may not be able to resolve accurate sharp moving fronts and corresponding groundwater flow velocities due to the numerical instabilities.
In this presentation, we employ the enriched Galerkin finite element methods (EG), which enriches a classical continuous Galerkin finite element methods with piecewise constant functions to ensure local and global mass conservation. EG has the same bilinear forms as the discontinuous Galerkin (DG) finite element methods but EG has fewer degrees of freedom in comparison with DG. Moreover, dynamic mesh adaptivity approaches are employed to save computational cost for realistic large-scale problems and an efficient Krylov solver with preconditioner is provided. We will present initial numerical results for existing benchmark problems to show efficiency and effectiveness of the proposed method in density-driven flow modeling.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 231

Enriched Galerkin for Darcy flow, reactive transport and elastic wave propagation

Mary Wheeler¹

¹ The University of Texas at Austin

Corresponding Author(s): mfw@ices.utexas.edu

In this presentation, we discuss enriched Galerkin (EG) algorithms for modeling Darcy flow, reactive transport, and elastic wave propagation. This approach involves enriching the continuous Galerkin finite element method with discontinuous elements. For transport EG is coupled with entropy residual stabilization for transport. The method provides locally and globally conservative fluxes, which are crucial for coupled flow and transport problems. In particular, numerical simulations of viscous fingering instabilities in heterogeneous porous media and Hele-Shaw cells are illustrated as well as results for two phase flow. Here dynamic adaptive mesh refinement is applied in order to save computational cost for large-scale three-dimensional applications. In addition, entropy residual based stabilization for high order EG transport systems prevents any spurious oscillations. Recently EG was applied to simulated elastic wave propagation in a fractured media. Here Linear Slip theory was used for incorporating fractures and faults. Specifically, this new approach has the advantage of DG with a computational cost comparable to that of the Spectral Element Method. Computational results demonstrating the effectiveness of EG for these flow and reactive transport and wave propagation are provided. The work on flow and transport was done in collaboration with Sanghyun Lee and the work on elastic wave propagation with Mrinal Sen and Janaki Vamaraju.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 229

Enriched Galerkin with Direct Serendipity Elements on Quadri-laterals for Two-Phase Flow in Porous Media

Author(s): Zhen (Jane) Tao¹
Co-author(s): Todd Arbogast ²

¹ University of Texas
² University of Texas at Austin
**Corresponding Author(s):** taozhen.cn@gmail.com

Enriched Galerkin (EG) methods were defined in 2009. The idea is to use a variational form arising from a discontinuous Galerkin (DG) method, but instead of using discontinuous approximating spaces, one uses a continuous space enriched with piecewise discontinuous constants. EG has fewer degrees of freedom than DG, and so is easier to solve, but it maintains the local conservation property of DG. On quadrilateral meshes, the natural choice is to use the tensor product polynomials defined on the reference square and mapped to the physical elements. These maintain accuracy under bilinear distortion. The classical serendipity finite element spaces have even fewer degrees of freedom, but they suffer from poor approximation on nondegenerate, convex quadrilaterals. We develop the direct serendipity spaces $\text{DS}_r$, a new family of finite elements for $r \geq 2$ that has the same number of degrees of freedom as the classical space but maintains optimal approximation properties. The set of local shape functions for $\text{DS}_r$ contains the full set of polynomials of degree $r$ defined directly on each element. Because there are not enough degrees of freedom, exactly two supplemental rational functions are added to each element. We use these new spaces in an EG method to solve flow and transport problems in porous media, including the saturation equation of two-phase flow. A partial extension to 3D will also be presented.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 10-F / 392**

**Estimating permeability of shale gas reservoirs from porosity and mineral contents**

**Author(s):** Peiqiang Zhao

**Co-author(s):** Zhenhua Huang ; Songcheng Tan

1. *Huabei Subsurface Multi-scale Imaging Key Laboratory, Institute of Geophysics and Geomatics, China University of Geosciences (Wuhan)*
2. *Chongqing Institute of Geology and Mineral Resources*
3. *Faculty of Engineering, China University of Geosciences (Wuhan)*

**Corresponding Author(s):** zhaopq@cug.edu.cn

Permeability is one of the most important petrophysical parameters for reservoir characterization, completion design and production prediction, etc. However, due to the strong heterogeneity, poor pore structure, extremely low porosity and complicated minerals types in shale gas reservoirs, it is challenges for estimating the permeability accurately. In this paper, we present a method for predicting permeability from porosity and mineral contents data. 30 samples drilled from the Lower Silurian Longmaxi shale formations, Sichuan Basin, China, were conducted to porosity, permeability, TOC contents and XRD analysis. Several samples were also used for nitrogen adsorption experiments to get the rock specific surface. We used the Kozeny’s equation to calculate the specific surface of the solid phase. The specific surface derived from the Kozeny’s equation, which is lower than that obtained from nitrogen adsorption, is view as an effective specific surface related to micro and macro pores. The specific surface obtained from the nitrogen adsorption is mainly attributed to the micro pores of shale rocks. The relationship between the effective specific surface and TOC and mineral contents have been analyzed. The effective specific surface are positively correlated with clay contents, but negatively correlated with other non-clay minerals. However, there is no correlation between the TOC and effective specific surface. This may be because the Kozeny’s equation method removes the TOC effect on porosity. Based on the analysis, an empirical equation between the effective specific surface and clay and several main non-clay minerals was established using weighted least square method to process the heteroscedasticity. Thus, the permeability can be predicted from porosity and mineral contents via the Kozeny’s equation. The results show that the predicted and measured permeability have a good agreement. The proposed permeability prediction method was applied to the field wells. The mineral contents
could be obtained from geochemical log data or calculated using conventional well logs with optimization method. Good applications were achieved, indicating the proposed method is effective and reliable.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 655

Evaluating the Potential of Nanoparticles for Foam Generation and Stability at High Temperatures: Steam Foam Application

Author(s): Adam Fehr¹

Co-author(s): Jelayne Falat ¹ ; Ali Telmadarreie ² ; Steven Bryant ³

¹ CERC Co-op Student
² Postdoctoral Research Fellow
³ Professor

Corresponding Author(s): steven.bryant@ucalgary.ca

Steam injection has been implemented with residual oil saturation in swept zones being as low as 10% in the case of Steam Assisted Gravity Drainage (SAGD) processes. The primary difficulty with a gas injection of any kind is conformance due to low density and viscosity of the gas. Therefore, gases tend to form channels and pathways through oil rather than displacing the oil. Traditionally foam-forming additives such as surfactants have been added to reduce gas mobility. However, the surfactants ability to perform under harsh conditions (e.g. temperature and salinity) are limited. Nanoparticles can be a promising enhancer/stabilizer for foam additives at reservoir condition. This is promising for EOR processes with steam (i.e. SAGD) since the increased mobility control and the transport stability, can improve the conformance control and consequently sweep efficiency.

In this study, the foam height tests (Nitrogen as the gas phase) were performed with the surfactants, nanoparticles, and combinations of the two with the help of high-pressure high-temperature (HPHT) visual cell. Foams generated with surfactant were treated as a baseline and effect of nanoparticle addition on foam behavior was studied. Dynamic light scattering was used to characterize all nanoluid solutions before and after foam height tests to ensure nanoparticle-surfactant compatibility and stability in solution at HPHT condition. After screening the various foaming agents, the dynamic flow experiments were performed with a specially configured core flood apparatus designed for steam foam flooding. Propagation of the nitrogen foam was measured using four differential pressure taps located along the length of the porous media (100 °C and 500 psig). In addition, steam foam flow experiments were also performed in the presence of nitrogen as a non-condensable gas (500 psig and 250 °C). Effluent samples were analyzed for nanoparticle and surfactant effective concentrations using high accuracy inductively coupled plasma triple quadrupole mass spectrometry that yielded retention and adsorption.

In initial foam height tests (500 psig and 100 °C) it was observed that the combination of a studied coated silica nanoparticle and sodium dodecylbenzenesulfonate surfactant produced foam with a better texture, and a longer retention of foam height compared to foam generated with the only surfactant. In addition, the foam produced with a proprietary nanoparticle alone outlasted the surfactant stabilized foam at HPHT condition. The increase in foam half-life was also correlated with higher mobility reduction and faster foam propagation in nitrogen and steam foam flow experiments. Effluent composition profiles and tracer composition profiles developed by ICP-QQQ analysis yielded mass balance data in addition to providing detailed information about the throughput of injection fluid. Dynamic flow experiments revealed the synergy between nanoparticle and surfactant in steam foam application (i.e. mobility control) compare to that of the steam-surfactant system. The results obtained through this study yielded data regarding multiphase transport of nanostructured foams through porous media at high temperatures, such as propagation through porous media, nanoparticle stability in harsh conditions, retention and adsorption of surfactant, nanoparticles, and their combinations. The knowledge obtained from this study significantly improves our understanding of nanoparticles as an additive in steam foam application.
Parallel 9-F / 618

Evaluation of Microbial-mediated Moisture Retention in Emulated Soil Micromodels

Author(s): Yi-Syuan Guo

Co-author(s): Jessica Furrer 2; Daniel Gage 1; Yong Ku Cho; Leslie Shor 1

1 University of Connecticut
2 Benedict College

Corresponding Author(s): yi-syuan.guo@uconn.edu

Pore-scale water content controls the function of soil microbial communities by modulating the hydraulic connectivity of microbial communities and the flux of aqueous and gaseous substrates. In turn, soil bacteria regulate local moisture within porous structure through the secretion of extracellular polymeric substances (EPS). EPS promotes water retention as hydrogel in several ways: (i) by increasing the abundance of intra-aggregate micropores via soil aggregation, (ii) by swelling during wet soil conditions and remaining hydrated during dry soil conditions, and (iii) by altering soil surface wettability. The complex microbial process of soil moisture regulation can be understood by controlling the micro-structured environment systematically. Here we describe pore-scale changes in moisture distribution within emulated soil micromodels featuring systematically varied physical microstructures and surface water repellencies, loaded with well-defined pore solutions. Air infiltration into initially water-saturated soil microenvironments was recorded and quantified using microscopy. Experimental results showed that microstructure geometry was found to effect drying rate over a range of pore saturation values as well as control the spatial distribution of liquid and gas phases with unsaturated soil micromodels. EPS was cultured from stationary-phase Sinorhizobium meliloti bacteria, and was diluted to 0.25x, or concentrated via lyophilisation to 5x. The pristine EPS solution took twice as long to dry compared with pure water in identical micromodels. The 0.25x EPS solution took about four times slower than deionized water, and the 1x EPS solution took about eight times slower than deionized water. The influence of a relatively small amount of EPS is magnified by the porous structure to limit evaporation at pore throats. These results illustrate how natural microbial processes work within a complex soil microstructure to control the spatial distribution of water and limit the loss of soil moisture. We provide a systematical method to evaluate drying process within realistic soil microenvironments; we anticipate our approach may facilitate development of novel agriculture biotechnology to enable farmers to produce more crops using less water.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 2 / 191


William Godoy1; Elizabeth May Pontedeiro2; Xiaoguang Yin2; Enno de Vries4; Fernanda Hoerlle3; Amir Raoof2; Paulo Couto5; José Santiago7

References:

Acceptance of Terms and Conditions:

Click here to agree
Heterogeneous carbonate rocks, especially coquinas, present several challenges regarding their morphological characterization, petrophysical parameterization, and obtained a more complete understanding of their fluid flow properties. Within this context, a workflow is proposed and analyzed for digital petrophysics using a combination of experimental data and numerical 3D fluid flow simulations. The proposed workflow is applied to coquinas (Brazilian Pre-Salt analogue carbonates) in efforts to evaluate their petrophysical properties.

The workflow involves basic petrophysics as well as state-of-the-art approaches in digital analyses, to characterize coquina samples. Outcrop coquina samples were for this purpose selected from the Morro do Chaves Formation in Northeastern Brazil, which has been studied as analogue rocks of Santos Basin Pre-Salt carbonates. Important steps in the workflow are the geological and morphological analysis of the selected coquinas samples (including basic petrography), acquisition of data through X-ray computed microtomography using different spatial resolutions, three-dimensional reconstruction and modeling of the coquinas and their pore systems, and numerical simulation of fluid flow in the porous media. Experimental data were obtained using permeametry, porosimetry, NMR, and SEM in support of several key steps of the workflow, such as segmentation procedures. Numerical simulations were used to estimate absolute and relative permeabilities using PNM- and FEM-based approaches. We used for this purpose commercial and in-house codes developed at both Utrecht University (Netherlands) and the University of Rio de Janeiro (Brazil).

All digital and numerical steps within the proposed workflow are being validated against experimental data to understand the limitations and uncertainties of the various steps. We highlight the main challenges and uncertainties encountered during each step, including challenges related to proper estimation of the microporosity of coquinas, and appropriate definition of the REV (Representative Elementary Volumes) based on mathematical and statistical analyses. The workflow identified several important issues related to the digital petrophysics experiments of the coquina samples, including major challenges to properly characterize the porosity and related PNM- and FEM-based fluid flow simulations. Conclusions from this study will enable improved tailoring and optimizations of digital petrophysics predictions of Brazilian Pre-Salt carbonate reservoirs, based on a well-structured workflow that is self-correcting when combined with a range of experimental data.

References:

Acceptance of Terms and Conditions:

Click here to agree

Evaporation from gas diffusion layers of proton exchange membrane fuel cells: a pore network study

Rui Wu

Shanghai Jiao Tong University

Corresponding Author(s): ruiwu@sjtu.edu.cn

Evaporation from porous media is of great interest to many research and engineering fields, such as recovery of volatile hydrocarbons from underground oil reservoirs, remediation of contaminant soils by vapor extraction, and water management in gas diffusion layers (GLDs) of proton exchange membrane fuel cells (PEMFCs). During runnig of PEMFCs, produced water may condense and fill open pores of the cathode GDL, which impedes the transport of reactant gas to the reaction sites and hence is adverse to the fuel cell performance. In particular, at low temperature environment, liquid in the GDL can freeze to form ice crystals, which will damage the GDL structure and deteriorate the
performance and durability of PEMFCs. To this end, it is necessary to remove residual liquid in the GDL after the shutdown of PEMFCs. A common method is to purge the dry gas into the gas channel (GC) of a PEMFC to remove liquid in the GDL through the evaporation mechanism. However, the gas purge is parasitic and consequently reduces the efficiency of PEMFCs. To reduce parasitic losses and increase the system efficiency, it is important to understand the detailed evaporative liquid removal from GDL during the gas purge.

In PEMFCs, the cathode GDLs are thin (~250 μm) and treated with hydrophobic agent PTFE. However, due to non-uniform distribution of PTFE, the treated GDLs usually show mixed wet characteristics, i.e., hydrophilic and hydrophobic pores coexist. To investigate evaporation from such thin porous media with mixed wettability, a pore network model is employed in the present study. The GDL is conceptualized as a pore network (PN) composed of cubic pore bodies connected by cylindrical pore throats. Initially, the PN is fully saturated with liquid water. Then dry gas is flowed into the GC, during which liquid in the PN is removed by evaporation. The gas flow in the GC is considered as a fully developed laminar flow. The vapor transport in the channel is described by the convection-diffusion equation. The vapor transport in the PN is dominated by the diffusion. Both viscous and capillary effects are considered for liquid flow in the PN. The "capillary valve" effect is also taken into account to illustrate the movements of gas-liquid menisci in the pores of PN.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-F / 371

Evaporation of bound and free water from drying cellulose fiber poultices

Author(s): Mohamed Nidal BEN ABDELOUAHAB
Co-author(s): Alban Gossard ; Stéphane RODTS ; Philippe Coussot

1 CEA Marcoule - Laboratoire Navier
2 CEA Marcoule
3 Univ. Paris-Est

Corresponding Author(s): mohamednidal.benabelouahab@cea.fr

One of the innovative application of cellulose fibers is the desalination of masonry structures in the field of architectural heritage conservation. Wet poultices, classically composed of cellulose fibers and clays, are coated on the porous material to be treated, and kept in place before being removed when dry. The efficiency of the process partly depends on the drying behavior of the poultice, but so far little is known concerning cellulose drying. Understanding drying properties of cellulose fibers poultices present a real challenge since, due to the complex porous properties of the medium, it may contain several types of water liable to evaporate successively or simultaneously, and it may deform significantly.

We followed the drying of cellulose poultices with Nuclear Magnetic Resonance (NMR). Different NMR sequences were used which provided the evolution of key parameters in time: 1) the water saturation distribution; 2) respective bound and free water content (through different NMR relaxation times); 3) the sample shape. From this information we identified the different regimes of drying of cellulose poultices in relation with their microstructure evolution.

In a first period, the sample remains saturated and bulk water evaporates at a constant rate. This induces an axial shrinkage of the sample. A second period starts once the maximum possible shrinkage is reached. Now air starts to penetrate the sample. However, the water saturation decreases almost homogeneously throughout the sample. The drying rate remains constant during this period too, as in a model porous medium. Finally, at the end these two periods, 90% of water (almost all the free water) initially in the poultice has been evaporated. Then a falling drying rate period starts, associated to the development of a dry front inside the sample (from the free surface), and the evaporation of bound water (adsorbed) in cellulose fibers. This period leads to a further shrinkage.
of the structure due to fibers shrinkage. We conclude that, due to their specific fibrous structure the drying of cellulose poultries is particularly efficient, as almost 100% of the free water initially in the sample may be evaporated at a constant rate.

References:


Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 919

Evolution of Particle Swarms Falling under Gravity in Fractures

Author(s): Chven Mitchell¹
Co-author(s): Laura Pyrak-Nolte ² ; Ludwig Nitsche ³

¹ Purdue University
² Purdue University - Department of Physics
³ University of Illinois at Chicago

Corresponding Author(s): mitch240@purdue.edu

Cohesive particle swarms have been shown experimentally to exhibit enhanced sedimentation in fractures for an optimal range of fracture apertures. In this optimal range, swarms travel farther and faster than a disperse (particulate) solution. This study aims to uncover the physics underlying enhanced sedimentation. Swarm behavior at low Reynolds number in a quiescent unbounded fluid and between smooth rigid planar and rough boundaries is investigated numerically using direct-summation, particle-mesh (PM) and particle-particle particle-mesh (P3M) methods – based upon mutually interacting viscous point forces (Stokeslet fields). Wall effects are treated with a least-squares boundary singularity method, which can also model realistic, measured profiles of wall roughness. Much of the sedimentation behavior of a swarm is similar to the behavior of a homogeneous liquid drop. Sub-structural effects beyond pseudo-liquid behavior (i.e., particle-scale interactions) are approximated by the P3M method much more efficiently than with direct summation. The non-spherical initial shape instability, which occurs as the swarm is introduced into a tank below the surface of an otherwise quiescent fluid, leads to the formation of a torus. The swarm can also bifurcate, which significantly retards its sedimentation. Inhibition of breakup by the presence of the walls, within some optimal range of apertures, seems to account for the phenomenon of enhanced sedimentation.

From the simulations, if the initial swarm geometry at release is unaffected by the fracture aperture, no enhanced transport occurs. The swarm velocity as a function of aperture increases monotonically until it asymptotes to the swarm velocity in an open tank. However, if the fracture aperture affects the initial swarm geometry, the swarm velocity does not exhibit monotonic behavior. When swarms are released between two parallel smooth walls in very small apertures, the swarm is forced to reorganize and quickly deforms, which results in dramatic reduction in swarm velocity. At large apertures, the swarm evolution is similar to that of a swarm in open tank and quickly flattens into a slowly moving torus. In the optimal aperture range, the swarm maintains a cohesive unit behaving similarly to a falling sphere. Swarms falling in apertures less than or greater than the optimal aperture range, experience a level of anisotropy that considerably decreases velocities. Unraveling
the physics that drives swarm behavior in fractured porous media is important for understanding particle sedimentation and contaminant spreading in the subsurface.

Acknowledgment: This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Geosciences Research Program under Award Number (DE-FG02-09ER16022).

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-E / 407

Evolution of Pore Structures of In-situ Oil Shale Pyrolysis Through Superheated Steam

Dong Yang¹ ; Zhiqin Kang¹ ; Lei Wang¹

¹ Taiyuan University of Technology

Corresponding Author(s): yangdong@tyut.edu.cn

In-situ recovery of oil shale is an internationally recognized clean and efficient technology for extraction kerogen from oil shale. The technology- in-situ inject superheated steam into oil shale to exploit its kerogen, is a totally new technology proposed by Taiyuan University of Technology. In the process of in-situ pyrolysis and oil gas exploration of oil shale, pores and fractures of oil shale are not only the seepage channels of injected hot fluid to reach interior of oil shale, but also the passages of the outflow of pyrolysis products to the production wells. Thus, Evolution characteristics of pore and fracture of oil shale are the key to the success of oil shale in-situ mining. A pilot study of large size (1700±4001000mm) oil shale in-situ mining is conducted by Taiyuan University of Technology in 2015-2016, proving the feasibility of in-situ mining. In this study, the pore characteristics of oil shale samples located in different zones between injection and production wells are measured and statistics. The results show:

Porosity both along the direction of horizontal bedding plane and the direction of perpendicular of bedding plane are greater than the initial oil shale porosity, 1.5%, while in horizontal the porosity exceeds 27.65% and in vertical the porosity is more than 26.08%. It shows that the superheated steam has great impact on the pore structure evolution.

After the pores being divided into four grous-micropores, small pores, mesopores and macropores according to the pore size, one can find along bedding planes, the proportion of four pore groups is varied as mesopore>small pore>macropore>micropore. The proportion of mesopore is the largest and is the most significant to total pore structure;

In the whole pyrolyzed zone in the sample, oil shale with porosity among 23%~31% sums up to 75%. The results compared to oil shale after direct pyrolysis by heat, the porosity is only about 20%, shows validating the feasibility of convection heating of oil shale.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-G / 676

Examination of Capillary Pressure-Saturation-Interfacial Area Relation under Dynamic Conditions using Volume-Of-Fluid (VOF) Method
Santosh Konangi¹; Nikhil Kumar Palakurthi¹; Nikolaos Karadimitriou²; Ken Comer³; Urmila Ghia¹

¹ University of Cincinnati
² University of Manchester
³ The Procter & Gamble Company

Corresponding Author(s): konangisantosh@gmail.com

Conventional two-phase flow equations (Richards Equation) for porous media at the macroscale require capillary pressure (Pc) and relative permeability (Kr) measured as a function of saturation (S). However, these equations lack solid theoretical foundation, and there is still a considerable gap between the theory and experiments. In typical experiments, an “average” macroscopic capillary pressure is measured as the difference between the pressures of the non-wetting-phase reservoir at the inlet and wetting-phase reservoir at the outlet of a porous medium. Traditionally, this macroscopic phase pressure difference is assumed to be equal to the pore-scale capillary pressure arising due to the curvature of the menisci at the fluid-fluid invasion front. Many theoretical and experimental studies have shown that the macroscopic definition is valid only at equilibrium (i.e. static conditions) and if the phases are connected (Ferrari et al., 2013). Under non-equilibrium (dynamic) conditions, when the fluids are moving, the dynamic capillary pressure measured in experiments is a combination of capillary pressure at the invasion front and the pressure head caused by viscous effects (Lovoll et al., 2011).

The Pc–S relationship is non-unique, and is flow process dependent; different Pc–S curves are defined for drainage and imbibition experiments, resulting in “hysteresis” (Joekar-Niassar and Hassanzadeh, 2012). Gray and Hassanzadeh (1991, 1993) developed a theoretical framework for unsaturated capillary flows which proposed that the inclusion of specific fluid-fluid interfacial area will explicitly define the state of the system, resulting in a unique relation between capillary pressure, saturation and interfacial area (Pc–Sw–awn). In this study, we investigate the capillary pressure–saturation relation under equilibrium and non-equilibrium conditions using pore-scale direct numerical simulations (DNS). Direct numerical simulations (DNS) allow for high resolution description of the geometry and time evolution of interfaces, thereby permitting us to investigate the uniqueness of transient Pc–Sw–awn surfaces.

The porous medium is represented by a quasi-two-dimensional flow network of cylindrical obstructions. Hex-dominant computational grids are generated to accurately resolve the inter-cylinder pore space. The Navier–Stokes (NS) equations are solved in the pore space on an Eulerian mesh using the open-source finite-volume computational fluid dynamics (CFD) code, OpenFOAM. The Volume-of-Fluid (VOF) method is employed to track the evolution of the fluid–fluid interface; a static contact angle is used to account for wall adhesion. Simulations of drainage and imbibition are performed for different capillary numbers by controlling the flow rate of the non-wetting (polydimethylsiloxane oil) and wetting (water) fluids. From these micro-scale simulations, the pore-scale capillary pressure is directly determined at the fluid-fluid invasion front; this capillary pressure depends on the pore morphology and interfacial energy at the fluid-fluid interface, without accounting for the viscous dissipation which is dependent on system size and invasion speed. The pore-scale capillary pressure is upscaled using the fluid-fluid interfacial area to estimate the macroscopic equilibrium (quasi-static) and non-equilibrium (dynamic) Pc–Sw curves; the Pc–S–awn surface is constructed to determine whether the data points from drainage and imbibition processes fall on a unique surface under transient conditions.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-B / 612

Experimental Investigation and Synchrotron Visualization of Water Transport of Thin Porous Media in Polymer Electrolyte Membrane Fuel Cells.

Author(s): Logan Battrell

Co-author(s): Prasaad Milner 1 ; Megan English 1 ; Lifeng Zhang 2 ; Ryan Anderson 1

1 Montana State University
2 University of Saskatchewan

Corresponding Author(s): logan.battrell@montana.edu

One of the key issues related to long-term polymer electrolyte membrane (PEM) fuel cell durability is water management within the porous gas diffusion layer (GDL). When too much water accumulates within the GDL, the flow of the gases to the catalyst layer becomes restricted, which can lead to the degradation of key cell components or even result in total cell failure. Therefore, understanding the water transport phenomena within the porous GDL is a key component to optimal fuel cell design. In this work, the characterization and visualization of water transport within the GDL of a PEM fuel cell is investigated from macro (e.g. fuel cell performance) and micro (e.g. pore scale) perspectives. Results from these experimental investigations are integrated into a computational fluid dynamics (CFD) model of water vapor transport across the membrane electrode assembly (MEA). At the macroscale, a novel technique is used to determine the effective diffusivity by experimentally measuring water transfer rates across an electrochemically active PEMFC. This technique expands upon a previously published anode water removal (AWR) diagnostic protocol, which functions to remove excess cathode GDL water. This protocol allows for the introduction of an evaporative gradient which drives water transport across the MEA into an initially dry anode stream. The strength of this gradient is controlled by the flow rate of the anode stream. In this work, the resulting relative humidity of the anode stream is determined through analysis of the anode pressure drop, allowing for the quantification of the water flux. This approach allows for a combined analysis of fuel cell performance and net water vapor transport. Through analysis of the water vapor transport rates and water concentrations of the anode and cathode streams, overall effective diffusivities are calculated during in-situ operation. However, at the macroscale the fuel cell components are opaque, making it difficult to resolve the water flooding issues locally. The lack of microscale data in the porous GDL hinders optimized operating conditions and material designs. To address this issue, synchrotron radiography is utilized at the Canadian Light Source to investigate and visualize GDL de-saturation at the micro scale. The high x-ray flux provided by synchrotron radiography allows for rapid x-ray computed tomography scans, which are used to visualize the transient de-saturation process. This ex-situ procedure mimics the desaturation that occurs in the macroscale tests. Two different GDL samples are investigated to determine the contributions of convection and evaporation, specific water removal pathways, and overall de-saturation rates. Results show that the major de-saturation mechanism is evaporation, but that convection also plays a minor role. Results agree with previous studies showing that water is removed preferentially under the channels, and then from underneath the ribs. An initial CFD model is developed based on the experimental fuel cell architecture to verify water transfer rates and effective diffusivities obtained in the macro study.

References:

1) Battrell, L., A. Trunkle, E. Eggleton, L. Zhang, and R. Anderson, Investigation of Water Transport Within a Proton Exchange Membrane Fuel Cell by Diffusion Layer Saturation Analysis. ASME. Interna-

Parallel 1-B / 166

Experimental Studies on the Hydraulic Effects of Fungal-Mycelia in Sandy Soil

Grainne El Mountassir1 ; Emmanuel Salifu2

1 University of Strathclyde, Glasgow, United Kingdom
2 University of Strathclyde Glasgow and Università di Napoli Federico II, Napoli

Corresponding Author(s): emmanuel.salifu@strath.ac.uk

One gram of soil can contain up to 100 million to 1 billion microorganisms and up to 1 million different species of microorganisms. Despite this fact, geotechnical engineers have, until fairly recently, ignored biological activity in the soil or possible biological amendments that could be introduced. Over the last ten years research has focused on bioaugmentation strategies (i.e. the injection of a single strain of bacteria) to alter hydraulic and mechanical behaviour of porous and fractured media (e.g. microbially induced calcite precipitation). One challenge of bioaugmentation technologies is the transportation of bacteria within the ground. This study investigates for the first time the potential use of fungal networks for ground engineering applications. Fungi produce hyphae, long filamentous structures which collectively are called a mycelium. Mycelium can grow to vast sizes, with individual mycelia (in forest floors) covering areas up to 9km² in North America. As such there is great potential ‘to grow’ fungal mycelia for earth infrastructure over large areas.

We investigated the hydraulic behaviour of sandy soils treated with fungal mycelia using P. ostreatus (oyster mushroom) in order to: (i) Assess the level of hydrophobicity induced and (ii) understand the influence of P. ostreatus mycelia on water flow through the soil profile. To investigate these, we grew mycelia in petri dishes and conducted water drop penetration tests to ascertain induced hydrophobicity. We also determined the surface water evaporation rates for soils with mycelia and those without, at different starting moisture conditions. Next, we set up a 1-dimensional infiltration column test with mycelia inoculated and incubated to grow overtime throughout the soil profile. The infiltration column was instrumented with tensiometers and Time Domain Reflectometer (TDR) probes for the real-time measurement of suction and water content. Soil infiltration water fronts were obtained for both treated and untreated soils in respective columns. The presence of fungal mycelia resulted in significantly altered hydraulic characteristics of the soils. Mycelia induced extreme hydrophobicity on fine sands and reduced surface water evaporation rates. Infiltration time was slower for fungal-treated soils than untreated soils. These results highlight the potential for fungal mycelia to be used in the creation of semi-permeable or impermeable barriers in a range of ground engineering applications.

Key words: fungal mycelia; soil hydraulics; ground improvement; 1-D infiltration;

References:

Acceptance of Terms and Conditions: Click here to agree

Poster 1 / 748
Experimental Study and Modeling of Biogas Formation in Homogeneous Porous Media

Daeyun Kim¹ ; Nariman Mahabadi¹ ; Jaewon Jang² ; Leon van Paassen¹

¹ Arizona State University  
² Hanyang University

Corresponding Author(s): dkim147@asu.edu

Biologically mediated processes are being developed as an alternative approach to traditional ground improvement techniques. Denitrification has been investigated as a potential ground improvement process towards liquefaction hazard mitigation. During denitrification, microorganisms reduce nitrate to dinitrogen gas and facilitate calcium carbonate precipitation as a by-product under adequate environmental conditions. The formation of dinitrogen gas desaturates soils and allows for potential pore pressures dampening during earthquake events. While, precipitation of calcium carbonate can improve the mechanical properties by filling the voids and cementing soil particles. As a result of small changes in gas and mineral phases, the mechanical properties of soils can be significantly affected. Prior research has primarily focused on quantitative analysis of overall residual calcium carbonate mineral and biogenic gas products in lab-scale porous media. However, the distribution of these products at the pore-scale has not been well-investigated. In this research, denitrification is activated in a microfluidic channel simulating a homogeneous pore structure. The denitrification process is monitored by sequential image capture, where changes in the gas and mineral phase are evaluated by image processing. The results from the experimental study are compared to the results of two-dimensional simulation model which involves the relevant biochemical reactions, diffusion, and convection.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 247

Experimental Study on seepage characteristics of sandstone affected by fracture surface roughness and fracture width

LIU Xiangfeng¹ ; REN Yanjin²

¹ Liaoning Technical University  
² China Construction Eighth Engineering Division Rail Transit Construction Co.LTD

Corresponding Author(s): 305066889@qq.com

In order to quantitatively describe the influence of the surface roughness of sandstone fracture on its seepage law, the three-dimensional fractal dimension D and three-dimensional surface height deviation Sa are used to characterize the surface roughness of sandstone fracture. Through the seepage test of sandstone specimen with different fracture surface roughness and different crack opening width, the influence of crack surface roughness and crack opening width on the seepage characteristics of sandstone is studied. Based on the ideal cubic law, the seepage model of rough fracture is established. The results show that the larger the surface roughness is, the larger the surface height deviation is, and the 3D fractal dimension D approaches 3. For the same rough fracture, the fracture seepage flow rate increase exponentially with the increase of the fracture opening width, and show obvious nonlinear characteristics. With the same fracture opening width, the seepage flow of the sandstone specimen is affected by the surface roughness of the fracture, and the surface roughness of the fracture is negatively correlated with the flow rate of the fracture seepage. The difference of the seepage flow in the low fracture width stage (50 ~175) is not obvious, The difference of the seepage flow in the high fracture width stage (175 ~300) is obvious; With the increase of the width of the fracture, the effect of the fracture surface roughness on the flow rate of the fracture is reduced. Through the dimension analysis method, the cubic law is improved, and the rough fractured flow...
model with 3D fractal dimension D is established, and there is a good agreement with the seepage law of sandstone fracture, model is more reasonable.

References:

Poster 3 / 207

**Experimental Study on the Effect of Moisture on Adsorption and Diffusion of Coalbed Methane**

**Author(s):** Wencheng Han¹

**Co-author(s):** Aifen Li ¹; Weibing Tian ¹; Qi Fang ¹; Shuaishi Fu ¹

¹ China University of Petroleum

**Corresponding Author(s):** hwencheng57@126.com

Adsorption is one of the most important ways of coalbed methane stored in the coal seam. Methane diffusion in coal plays an important role in coalbed methane production. Understanding the characteristics of adsorption and diffusion of coalbed methane is keys to correctly evaluate the gas content and effectively enhance the gas production. As well known, most coal seams contain a certain amount of moisture. Its influence on methane sorption and diffusion should be considered in studies of coalbed methane content estimation and gas production prediction. To investigate the effects of moisture on adsorption and diffusion of coalbed methane, isothermal adsorption experiments of coal samples with different water contents at different temperatures and pressures were carried out. The “stretched exponential” model which couples a characteristic rate parameter kφ with a stretching parameter β was adopted to calculate the diffusion coefficient by using the data of adsorption experiments. The results show that the methane adsorption obey the adsorption model of “Dubinin-Astakhov-k” for all dry coal samples and moist coal samples the methane adsorption capacity was decreased with the increase of water content, meanwhile, the diffusion coefficient in the moist coal samples is much lower than the diffusion coefficient in the dry coal samples, which mean that the water hinders the gas transportation in the pores of coal obviously. Moreover, increasing the temperature can decrease the methane adsorption capacity and enhance the diffusion of gas for all dry samples and moist samples.

Keywords: moisture; adsorption; coal; stretched exponential; diffusion

References:

Poster 4 / 248

**Experimental Study on the Variation of Micro structure of Coal under Chemical Solution**

WANG Laigui¹; AN Wenbo¹

¹ Liaoning Technical University
Corresponding Author(s): 1611525041@qq.com

Coal is a low permeability solid medium with pores and fracture structures. Pore penetration affects the coal seam permeability. In order to damage the porous structure of coal to achieve the purpose of increasing penetration, X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR) were used to study the changes of mineral composition, mineral crystal particle size, morphology and bonding state before and after chemical solution immersion. The microscopic pore structure changes of coal before and after immersion in chemical solution were studied by means of scanning electron microscope (SEM) and mercury intrusion porosimetry test (MIP). The laws of the physical and mechanical properties of the coal were studied through the longitudinal wave velocity and uniaxial compression experiments before and after immersion in chemical solution. The mechanism of chemical damage of coal was discussed, and the damage evolution model of coal was established under chemical solution. The results show that: after chemical reaction, the content of carbonate minerals in coal decreased, the content of clay minerals increased and the mineral cement became loose. The microscopic pore size increased, and the porosity increased, the pores interpenetrate and the longitudinal wave velocity decreased. The mechanical properties of coal have the tendency to change from brittle failure to ductile failure. The damage of chemical solution to the structure of coal is a cumulative damage process from micro-destruction to macro-degradation. Mainly by the chemical effects caused (including dissolution, hydrolysis, ion exchange and adsorption and desorption, etc.)

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 220

Experimental analysis of tissue growth in a perfusion bioreactor

Author(s): Claire Beauchesne 1
Co-author(s): Morgan Chabanon 2; Bertrand David 3; Benoit Goyeau 4

1 CentraleSupelec
2 University of California, San Diego
3 CNRS
4 Centrale-Supelec

Corresponding Author(s): claire.beauchesne@centralesupelec.fr

Tissue engineering consists in combining an absorbable scaffold with cells of interest and the proper culture medium in order to produce a tissue for medical purpose. In particular, bone tissue engineering steps in as a promising alternative to the current reference treatments auto and allografts.

The objective is two-fold: first, to understand how fluid flow in the porous scaffold of the bioreactor influences tissue growth, especially considering bead packing heterogeneities. We considered the specific behavior at the periphery and in the core of the porous scaffold. Second, to tackle the main mechanisms of tissue growth formation.

The most striking cell response to mechanotransduction [3] is the formation of a peripheral envelop around the beads packing, as a consequence of the well-described flow channeling effect [4]. More generally, local numerical simulations allowed us to understand the regions where the cells where more likely to proliferate. Further observations of the microCT images and histology slides of the tissue grown on two different materials and at different culture times allowed us to identify the main mechanisms of tissue formation, development and reorganization in the bioreactor.

References:


Acceptance of Terms and Conditions:

Click here to agree

---

**Poster 4 / 132**

**Experimental and Numerical Studies of Saturation Overshoot during Water Infiltration into Dry Soil**

Luwen Zhuang

S. Majid Hassanizadeh

C.J. van Duijn

1 Utrecht University

Corresponding Author(s): Lzhuang@uu.nl

Gravity-driven water flow into an initially dry porous medium can lead to a non-monotonic behavior. Instead of a uniform flow front, water infiltrates in finger patterns, which has been observed experimentally [1, 5, 4]. Fingering effect cannot be described by the Richards equation or standard two-phase flow system unless some additional terms are incorporated. One of the most effective approaches to model the observed saturation and pressure overshoot is to include the so-called non-equilibrium capillarity effect. Besides it, capillary or relative permeability hysteresis between imbibition and drainage processes also plays a key role in the degree of nonmonotonicity and its pattern.

In this work, we first performed a series of one-dimensional water infiltration experiments in dry soil. The experiments were conducted with different water flow rates and different initial saturations. Saturation was measured at one location using the gamma-transmission method, while water pressures were measured at multiple locations during the experiments. We employed two alternative approaches, referred to as the extended-standard (ESD) model and interfacial area (IFA) model, to simulate the experimental results.

References:

Acceptance of Terms and Conditions:

Click here to agree

---

**Poster 3 / 201**

**Experimental and simulation research on the influence of temperature on the porous and thermal properties of sandstone**

Haiyuan Yang

Yongfei Yang

1 China University of Petroleum (East China)

2 China University of Petroleum (East China)

Corresponding Author(s): yanghaiyuun@icloud.com

In the process of thermal recovery and the underground storage of nuclear waste, the porosity and permeability of rock will change significantly from thermal stress. In this paper, a sandstone sample was subjected to heating, porosity examination, permeability measurements and CT scanning.
Based on digital core technology, permeability and thermal conduction simulations were performed. The results show that due to the discontinuity character of thermal cracking, as the temperature increases, the permeability of sandstone increases with fluctuations, resulting in a final value that is higher than the initial value. The permeability of the pore network model is fit to the experimental permeability, whereas the fractal model exhibits a closed relationship with the pore throat diameter. The thermal conductivity simulation shows that due to the porosity’s changing with the temperature, the thermal conductivity coefficient exhibits an opposite fluctuating change.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 1107

Experimental investigation on self-generated heat foam system for offshore heavy oil reservoir

Hailong Chen\textsuperscript{1}; Zhaomin Li\textsuperscript{2}; Wang Fei\textsuperscript{2}; Haifeng Li\textsuperscript{3}; Kang Yang\textsuperscript{3}; Meijia Wang\textsuperscript{3}

\textsuperscript{1} China University of Petroleum
\textsuperscript{2} Geo-Energy Research Institute, Faculty of Electromechanical Engineering, Qingdao University of Science and Technology
\textsuperscript{3} College of Petroleum Engineering, China University of Petroleum

Corresponding Author(s): chenhailong0515@163.com

Foam fluid is a gas-liquid dispersion system whose range of application covers various fields due to its excellent properties, especially in oil and gas field development including enhanced oil recovery, matrix acidizing, gas breakthrough control, profile control, plugging removal, etc. However, factors such as dependence on natural N2 sources, breakthrough of N2 to production wells, transportation of N2 and field equipment, environmental problems and safety have restrained broad use of the N2 foam injection technique in offshore reservoir.

To overcome these issues and extend the application of foam fluid, a new method, namely, underground foaming method, should be used to replace the conventional foaming method and the foam should carry heat. In this paper, we used a self-generated heat system (SGHF) to achieve this goal. The technique is based on the injection of two aqueous solutions i.e. gas-forming and gas-yielding solutions of certain concentrations into the reservoir. In this research, SGHF was obtained by a chemical reaction between gas forming ammonium chloride and sodium nitrite and the reaction products are very friendly, which are N2 gas, H2O, NaCl, and heat. This system has been studied and used in petroleum engineering.

In this work, we firstly perform surfactant evaluation experiments to identify the temperature resistance and salt resistance surfactant suitable for application conditions of offshore reservoirs. Then, we carried out sandpack flooding experiment including single sandpack flooding experiment and parallel sandpacks flooding experiment, as well as the 2 dimension visualization model experiment of three different research systems (SGHF systems, self-generate heat (SGH) system and conventional foam system) to study and analyze the enhancing oil recovery mechanisms of SGHF system. After analyzing and discussing the experimental results including trap gas volume analysis, calculation of internal chemical reaction degree in sandpack, temperature distribution inside sandpack and temperature variation coefficient, we draw the conclusion that the main mechanisms of enhancing oil recovery are(1) SGHF system can generate more uniform and even foam than the conventional foam, which not only eliminate the need of gas resource and gas transport, but also provide better gas fluidity control and adjust the production profile of heterogeneous reservoirs. (2) Foam can adjust the temperature distribution. Temperature distribution inside the sandpack is relatively uniform and high for SGHF system which benefits to reduce the viscosity of heavy oil in a larger scale, and we think the reasons are mainly including: Firstly, the presence of foam and the properties of trap gas cause the gas to accumulate near the inlet area, the effective permeability at the inlet decreases, therefore, the reaction heat production is performed evenly in the front and rear parts. Secondly, the presence of a large amount of trapped gas in the sandpack reduce the overall thermal conductivity inside the sandpack and delays the loss of heat.
Experimental investigations of effective visco-elastic properties of sandstones

Jana Musialak\(^1\); Jörg Renner\(^2\); Holger Steeb\(^3\)

\(^1\) University of Stuttgart & Ruhr-Universität Bochum
\(^2\) Ruhr-Universität Bochum
\(^3\) University of Stuttgart

Corresponding Author(s): holger.steeb@mechbau.uni-stuttgart.de

The effective visco-elastic properties of reservoir rocks are strongly dependent on characteristics of the pore geometry and of the inherent viscous pore fluids, saturation degree and excitation frequency. Constraining these dependencies is important for the interpretation of seismic data from geothermal or oil and gas reservoirs. Thus, experimental studies are needed that focus on effective visco-elastic properties in the frequency range of seismic field data. For this purpose, some laboratory apparatuses were developed in the past, using the forced oscillation method, in which stress and strain of a harmonically loaded sample are recorded and analyzed. In most of these studies, Young’s modulus and seismic wave attenuation were measured at frequencies below 100 Hz (e.g., [1-4]). However, to interpret complete seismic surveys, laboratory data are required up to even higher frequencies. Therefore, we developed a forced oscillation setup aiming at measuring the effective visco-elastic properties of partially and fully saturated rock samples in the seismic frequency range up to 1 kHz. Cylindrical samples are excited to axial oscillations during which the axial force and the axial as well as the lateral strain of the sample are measured to derive Young’s modulus and Poisson’s ratio and the two corresponding attenuation coefficients by a sliding-window fast Fourier transformation.

We present forced-oscillation experiments with varying amplitude (amplitude sweep) or frequency (frequency sweep) on different materials at ambient conditions. Calibration experiments were performed on visco-elastic polymethyl methacrylate (PMMA), commonly called Plexiglas, and elastic AlCuMgPb-alloy. These well characterized standard materials with contrasting behavior were already used to test similar apparatuses (e.g., [1-4]). The determined visco-elastic properties do not vary with amplitude in the investigated axial strain range of 4e–06 to 5e–05 (PMMA) or 3e–07 to 5e–06 (AlCuMgPb-alloy), but show a frequency dependence for PMMA. For example, the Poisson’s ratio of PMMA decreases continuously with increasing frequency, in agreement with previously reported trends [2]. Currently, we perform forced-oscillation experiments on samples of Berea sandstone with a porosity of approximately 18 %. The axial strain range, in which the four mentioned visco-elastic properties show no amplitude dependence, is identified in amplitude sweeps and used in the subsequent frequency sweeps.

References:

Poster 3 / 1007

Experimental study of turbulent flow over and within cubically packed walls of spheres: effects of permeability and wall thickness

Taehoon Kim¹ ; Gianluca Blois² ; James Best¹ ; Kenneth Christensen² ; Yaofa Li²

¹ University of Illinois a Urbana Champaign
² University of Notre Dame
³ University of Illinois at Urbana Champaign

Corresponding Author(s): yli26@nd.edu

Results of high-resolution particle velocimetry (PIV) measurements are presented to explore how the turbulent flow overlying a permeable wall is linked to the underlying pore flow and how their interplay is controlled by the topography of the wall interface and by the wall thickness. Two permeable walls were constructed from uniform spherical elements (25.4-mm diameter) in a cubically packed arrangement (porosity ~ 48%): one with two layers and the other with five layers of spheres. In addition, an impermeable rough wall with identical topography was considered as a baseline of comparison in order to explore the structural modifications imposed by permeability in the near-wall region. First- and second-order velocity statistics provide a quantitative assessment of such modifications of the local flow. A double-averaging approached allowed investigation of the global representation of the flow and assessment of conventional scaling parameters. A momentum deficit in the first pore layer and subsequent recovery beneath is observed, consistent with previous studies, as is a decay of the turbulent fluctuations. The transitional layer resides at the wall interface where free flow and pore flow interact, exchanging mass and momentum through intermittent turbulent events. Statistical investigation based on conditional averaging reveals that upwelling and down-welling flow events are associated with the passage of large-scale, low and high streamwise momentum free flow near the wall, respectively.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-B / 795

Exploring the limits of macro-homogeneous models of carbon-fiber papers

Pablo Ángel García-Salaberrí¹ ; Jeff Thomas Gostick²

¹ Universidad Carlos III de Madrid
² University of Waterloo

Corresponding Author(s): pagsalab@ing.uc3m.es

Carbon-fiber papers (CFPs) are an integral component of many energy-conversion and energy-storage technologies, including gas diffusion layers (GDLs) in polymer electrolyte membrane fuel cells (PEM fuel cells), cathode GDL in PEM electrolyzers and metal-air batteries, and as electrodes in redox flow batteries (RFBs). CFPs must fulfill several functions such as providing adequate mechanical support to the membrane electrode assembly, a transport pathway for reactants/products through its pore volume, and electrical and thermal conductivity through its solid fibrous structure. In RFBs, they have the added functionality of providing an active catalytic surface area. Understanding of the transport processes that occur in CFPs is necessary to help predict cell performance and durability, optimize materials and diagnose problems. The most common technique used to model these thin
porous media is the macro-homogeneous approximation based upon the existence of a representative elementary volume (REV). However, the applicability of the continuum approach to CFPs has been questioned many times, and the error introduced in the predictions is certainly unclear.

In this work, the limitations of macro-homogeneous descriptions of CFPs are explored for various single-phase transport processes: diffusion, convection and electrical/thermal conduction. Multiple sub-domains with different widths and thicknesses are examined by combining the lattice Boltzmann method with X-ray tomography images of uncompressed CFPs. The results show that a REV cannot be defined due to the lack of a well-defined separation between pore and volume-averaged scales in these inherently thin heterogeneous materials. The representative size in the material plane is in the order of 1 mm, which is comparable to the rib/channel width used in the above-mentioned devices. As for the through-plane direction, no representative length scale smaller than the thickness can be identified. In particular, it is found that the highly porous surface region (amounting up to 20% of the material) can significantly reduce the through-plane electrical/thermal conductivity.

In the second step, fuel cell performance predictions using a pore-scale model are compared to a traditional macro-homogeneous model. The results show that the overall mass, heat and charge fluxes predicted by both models are similar, provided that the macro-homogeneous model is equipped with suitable effective properties. However, the spatial distributions can be significantly different due to the lack of separation of scales. Specifically, the pore-scale simulations reveal the presence of inhomogeneities in the transport of species and heat that are not accounted for by the macro-homogeneous model. These deviations could have a substantial impact when modeling degradation phenomena, which are sensitive to local conditions.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-D / 986

Fast Evaluation of Rock Permeability from Images using Physics-Based Simulations and Machine Learning

Jinlong Wu¹ ; Xiaolong Yin² ; Heng Xiao³

¹ Virginia Tech
² Colorado School of Mines

Corresponding Author(s): xyin@mines.edu

Physical properties of rocks such as permeability, relatively permeability, and dispersion coefficient are of critical importance for prediction of subsurface flow and transport. Advances in microscopic imaging have made it possible to obtain the pore-scale microstructure of rock samples via SEM, TEM, or CT scan at low costs and fast turn-around time. Image-based reconstructions have also opened the door for obtaining rock characteristics by using physics-based pore-scale simulations. Unfortunately, such simulations are expensive, and as a result there are generally far more images than that can be simulated with current simulation technology and computational resources. A scheme for fast and accurate evaluation of physical properties of rock samples is urgently needed. In this work, we propose a computational framework and a workflow to evaluate permeability of rock samples by combining physics-based simulations and novel machine learning techniques. The computational framework fully utilizes the data provided by the lattice Boltzmann simulations while encoding the fundamental physics of flow in porous media into the architecture of the machine-learning model. The proposed framework is extensively evaluated on samples of a wide range of porosities and surface area ratios. Comparison of machine learning results and the ground truths suggest excellent predictive performance across all regimes, ranging from largely homogeneous pore structures to those with significant heterogeneities. The computational costs are reduced by several orders of magnitude compared to traditional simulations, demonstrating a great potential of the proposed framework.
**Poster 1 / 489**

**Fast assessment of CO2 plume extent using a connectivity-based surrogate model**

**Author(s):** Hoonyoung Jeong

**Co-author(s):** Alexander Sun

1 *University Of Texas At Austin*

2 *Bureau of Economic Geology, Jackson School of Geosciences, The University of Texas at Austin*

**Corresponding Author(s):** dragory@gmail.com

In a geological carbon storage (GCS) project, it is critical to predict the extent of injected CO2. However, it is not practical to quantify the uncertainty in the CO2 plume extent by conducting full physics flow simulations for hundreds of geological models representing high geological uncertainty. In this study, a computationally efficient surrogate model is introduced to quickly approximate CO2 plume migrations in a 3-dimensional heterogeneous reservoir during an injection period. CO2 plume migrations are approximated based on connectivities between a CO2 injector and other locations, which are computed using rock and fluid properties. The connectivity-based surrogate model saves about 90% of the computational cost in quantifying the uncertainty in the extent of CO2 plume compared to a full physics flow simulator.

**References:**

Click here to agree

---

**Poster 2 / 726**

**Fast large-scale joint inversion for deep aquifer characterization using pressure and heat tracer measurements**

**Author(s):** Jonghyun Lee

**Co-author(s):** Amalia Kokkinaki; Peter Kitanidis

1 *University of Hawaii at Manoa*

2 *University of San Francisco*

3 *Stanford University*

**Corresponding Author(s):** jonghyun.harry.lee@hawaii.edu

Characterization of geologic heterogeneity is crucial for reliable and cost-effective subsurface management operations, especially in problems that involve complex physics such as deep aquifer storage of carbon dioxide. With recent advances in computational power and sensor technology, large-scale aquifer characterization using various types of measurements has been a promising approach to achieve high-resolution subsurface images. However, large-scale inversion requires high, often prohibitive, computational costs associated with a number of large-scale coupled numerical simulation runs and large dense matrix multiplications. As a result, traditional inversion techniques have
limited utility for problems that require fine discretization of large domains and a large number of measurements to capture small-scale heterogeneity, like CO2 monitoring in the subsurface.

In this work, we apply the Principal Component Geostatistical Approach (PCGA), an efficient inversion method, for large-scale aquifer characterization. The domain considered is a synthetic three-dimensional deep saline aquifer intended for CO2 storage with 24,000 unknown permeability gridblocks. Transient pressure and heat tracer measurements from multiple dipole pumping tests are simulated with the TOUGH2 simulator and are used to estimate the heterogeneous permeability field and the corresponding uncertainty. For this scenario, we investigate the worth of combining heat and pumping tracer data for characterization. We demonstrate that with the PCGA, the inversion can be performed at a reasonable computational cost, while also resolving the main features of the permeability field. This presents opportunities for using inverse modeling to improve monitoring design and data collection strategies in field applications.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 545

Field-scale modelling of nanoparticle injection and transport for nanoremediation design and particle fate assessment

Tiziana Tosco\textsuperscript{1} ; Carlo Bianco\textsuperscript{1} ; Rajandrea Sethi\textsuperscript{1}

\textsuperscript{1} DIATI, Politecnico di Torino

Corresponding Author(s): tiziana.tosco@polito.it

The design of a field-scale injection of engineered nanoparticle (NP) suspensions for the remediation of a polluted site requires the development of quantitative predictive models for the system design and implementation.

In general, micro- and nanoparticle transport in porous media is controlled by particle-particle and particle-porous media interactions, which are in turn affected by flow velocity and pore water chemistry. During the injection, a strong perturbation of the flow field is induced around the well, and the particle transport is mainly controlled by the consequent sharp variation of pore-water velocity, and by the hydro-chemical properties of the injected fluid. Conversely, when the injection is stopped, the particles are transported solely due to the natural flow, and the influence of groundwater geochemistry (ionic strength, IS, in particular) on the particle behaviour becomes predominant. Pore-water velocity and IS are therefore important parameters influencing particle transport in groundwater, and have to be taken into account by the numerical codes used to support nanoremediation design. Several analytical and numerical tools have been developed in recent years to model the transport of colloidal particles in simplified geometry and boundary conditions. For instance, the numerical tool MNMs was developed by the authors of this work to simulate colloidal transport in 1D Cartesian and radial coordinates. Only few simulation tools are instead available for 3D colloid transport, and none of them implements direct correlations accounting for variations of groundwater IS and flow velocity.

In this work a new modelling tool, MNM3D (Micro and Nanoparticles transport Model in 3D geometries), is proposed for the simulation of injection and transport of nanoparticle suspensions in generic complex scenarios. MNM3D implements a new formulation to account for the simultaneous dependency of the attachment and detachment kinetic coefficients on groundwater IS and velocity. The software was developed in the framework of the FP7 European research project NanoRem and can be used to predict the NP mobility at different stages of a nanoremediation application, both in the planning and design stages (i.e. support the design of the injection plan), and later to predict the long-term particle mobility after injection (i.e. support the prediction of final fate of the injected particles). The application of the model in the framework of a novel approach for risk assessment at particle-contaminated sites is also reported.

References:
Parallel 3-B / 553

Filter media design for Dust Holding Capacity by computer simulations

Author(s): Mehdi Azimian ¹; Christopher Kühnle²
Co-author(s): Sven Linden ¹; Andreas Wiegmann ²

¹ Math2Market GmbH
² Math2Market

Corresponding Author(s): sven.linden@math2market.de

The goal of this study is to optimize a dual-fiber filter media by increasing the dust holding capacity (DHC), while maintaining the initial pressure drop and initial filter efficiency. Three main parameters define the performance of a filter, namely the DHC, filter efficiency and pressure drop. The DHC defines the quantity of solid particles which a filter media can trap and hold before the maximum allowable pressure drop is reached. The key idea is the use of micro structure models to optimize the filter media. To generate various filter media, the FiberGeo module of GeoDict® software is used, while the FlowDict and FilterDict modules simulate the flow behavior and the particle filtration behavior of the media, respectively.

Three different dual-fiber filter media are modelled. They all consist of the same two types of glass fibers (bi-modal diameter distribution). The distribution of the coarser fibers is uniform for all three models. They provide stiffness to the media and support the finer fibers. However, the finer fibers are distributed differently over the through-direction of the filter media [2]. The three models are called homogeneous model, linear increasing model, and exponentially increasing model. The naming scheme is based on the distribution of the finer fibers in through-direction of the filter media. In order to make the three models comparable, they were designed to have the same pressure drop in the clean state and to have the same initial filter efficiency. To ensure this, FlowDict and FilterDict simulations were used to guide the choice of geometric model parameters.

The first simulation step is to model the filter media with different spatial distributions of the two types of fibers. The next step is to simulate the clean fluid flow through the filter media. The final step is to simulate the particulate flow and particle deposition.

Filtration simulations on the three different models were done using the FilterDict module of GeoDict®. Filter life time simulations were carried out using the multi pass mode. In a multi pass simulation, fluids move in a circuit through the system, and the particle size distribution and concentration in front of the filter change over time. Outputs of these simulations are pressure drop, filtration efficiency and count/mass of the deposited dust as a function of time. The results show that by changing the distribution of the thin fiber type over the through-direction, the DHC of the filter media changes as well. In this way, the structure of the dual-fiber filter media can be optimized to achieve higher DHC, while keeping the initial pressure drop and initial filter efficiency the same.

References:


Click here to agree
Parallel 5-B / 552

First and second order transition during water adsorption in hemicellulose and its consequence on hygro-mechanical behavior

Chi Zhang¹ ; Dominique Derome² ; Jan Carmeliet¹

¹ ETH Zurich
² Empa

Corresponding Author(s): chi.zhang@empa.ch

Arabinoglucuronoxylan (AGX) is one of the most abundant hemicellulose of softwood. It is formed by β-1,4-linked β-D-Xylp units, partially substituted at O-2 by 4-O-Me-α-D-Glc-pA and at O-3 by α-L-Araf. It has diverse potential use in many industries, such as packaging of cosmetic or pharmacy, plastic additive and bio-refinery.

Despite its versatile potential, most of the key properties of xylan remain mysterious as it is difficult to isolate this polymer from wood sources without chemically altering it. Hemicellulose interacts strongly with moisture and induces many physical or mechanical changes. In this study, we apply molecular dynamics to investigate the mechanism of moisture influence on AGX. Moisture induces various changes to AGX, such as isotropic swelling, enhancing diffusion, shifting pore size distribution, decreasing stiffness, etc. Besides the first order changes of properties upon moisture adsorption, there also exists a second order transition which means that properties considered as function of moisture develop two regimes separated by a transition zone. Water population distribution analysis shows that multi-layer adsorption is the mechanism of the second order transition. Moreover, we show that the main polymer of wood, e.g. amorphous cellulose (AC), does not show such second order transition as AC is more water miscible compared to AGX.

References:

Acceptance of Terms and Conditions:

Click here to agree

---

Parallel 5-G / 823

Flow Behavior of Sheared Foam in Porous Media: An Experimental Investigation on the Effects of Stabilizing Agents and Oil Presence

Ying Yu¹ ; Zachary Soukup¹ ; Soheil Saraji¹

¹ University of Wyoming

Corresponding Author(s): yyu3@uwyo.edu

In enhanced oil recovery, foam is used for its inherent capability to act as a mobility control agent. Compared to conventional displacement fluids, such as surfactant and polymer solutions, foams contain up to about 95% less water, have tunable rheological characteristics, and leave behind less residue. However, foams are thermodynamically unstable, especially when exposed to hydrocarbons, and must therefore be treated with stabilizing agents.

This study focuses on the systematic characterization of nitrogen-foam rheology using steady-state and oscillatory shear measurements as well as core flooding tests. We investigate the effects of surfactant and salt concentration as well as additives, such as polymers and nanoparticles. Furthermore, the effects of different oils (n-Decane; Solvot 170; and Ekofisk crude oil) are investigated. In this study, foam is made by either sparging gas through a porous frit into aqueous surfactant solution or co-injecting gas and surfactant into a novel foam generator. The foam generator creates fresh, homogeneous foam by co-injection of up to three phases with highly controllable flow rates. This allows for the characterization of generative and destructive foam dynamics (by co-injecting an oil
phase) inside porous media. Berea sandstone with average porosity and permeability of 21.03% and 449.6 mD is used for the core flooding tests.

We find that higher concentrations of surfactant and/or salt containing monovalent counterions could enhance foam rheology, most likely due to a change in the rate of surfactant adsorption at the liquid-vapor interface. Furthermore, for a constant gas-volume fraction (91%), we show that a polymer additive could boost foam rheology if the gas phase is well dispersed in the surfactant/polymer solution and the bubble size that is produced decreases, thereby increasing the total surface area and multiplying the effects of enhanced film elasticity. Likewise, for the core flooding tests, we notice that polymer-enhanced foam increases the mobility reduction factor over polymer solution as injection rate increases and average bubble size decreases; though this corollary in porous media is better explained by the injection of pre-generated foam and elimination of any region of net foam generation inside the core. Moreover, contrary to reported observations of CO2-foam, nanoparticles have no appreciable effect on nitrogen-foam rheology, a discrepancy we believe to be a consequence of gas solubility and a slower rate of inter-bubble gas diffusion for N2 compared to CO2. On the other hand, as expected, oil has a considerably destructive effect on foam, and different oils lead to varying degrees of destabilization. In agreement with previous observations, foam is generally more stable in heavy oil than in light oil. However, a slight reversal of this trend in the three-phase core flooding tests as compared to the standard rheological measurements at atmospheric conditions hints at the added complexity of the fourth (solid) phase and the dynamic effects that arise during flooding in porous media. We believe the novel method of foam generation is more representative of the foam flooding process in oil reservoirs and could help in better understanding the dynamics of foam generation, destruction, and regeneration in porous media.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-B / 573

Flow and Mechanics in Fractured Media as Mixed-Dimensional PDEs

Wietse Boon1; Jan Nordbotten1

1 University of Bergen

Corresponding Author(s): wietse.boon@uib.no

In the mixed-dimensional representation of fractured media, the fractures are considered as lower-dimensional manifolds. This concept is successively applied to the lines and points at the intersections between fractures leading to a hierarchical geometry of manifolds of codimension one. By imposing these modelling assumptions a priori in the continuous setting, a basis is formed for the introduction of coupled PDEs on the mixed-dimensional geometry, which we refer to as mixed-dimensional PDEs.

In this work, we consider Darcy flow combined with linear elasticity on mixed-dimensional representations of fracture networks. Since the associated, governing equations are fully coupled, the systems of equations are presented using mixed-dimensional differential operators which map between the different dimensions. In turn, the resulting system of equations is considered as mixed-dimensional and can be analysed as such, before the introduction of the discretization scheme.

We present theoretical results related to the structure of mixed-dimensional elliptic partial differential equations from which multiple conforming discretization schemes arise using dimensionally hierarchical finite elements.

Keeping later purposes such as transport problems and fracture propagation in mind, our main interest lies in obtaining accurate flux fields and stress states which respect physical conservation laws. Therefore, we employ mixed finite elements which allow for a local preservation of such laws.
The symmetry of the stress tensor is imposed in a weak sense, thus leading to the use of familiar, conforming, finite elements with relatively few degrees of freedom.

Results concerning convergence and stability of the mixed finite element schemes are shown. These are supported by numerical examples in two- and three-dimensional domains in which the lower-dimensional inclusions, intersection lines, and points have significantly different material properties compared to the surroundings.

References:

Acceptance of Terms and Conditions:

Click here to agree

Invited 4 (Room B) - Parisa Mirbod / 1119

Flow and transport of particle-laden liquids over permeable surfaces; Theory and experiment

Parisa Mirbod

1 Clarkson University

Corresponding Author(s): pmirbod@clarkson.edu

The particle-laden liquids and their interaction with a permeable medium are important in various industries. However, research into their interaction has been bifurcated into two independent directions: suspension flows in geometries with smooth surfaces and flows of pure Newtonian fluids over porous media. Derivation of experimentally validated models and theory, which predict their coupling behavior and allow exploration of the impact of parameters from both suspension and porous medium are important.

In this seminar, I will present the steps made to comprehensively address the motion of suspension flows over permeable surfaces inspired by the almost frictionless movement of red blood cells through microvessels/capillaries. I will highlight two aspects of my group’s recent work that aim to understand the interrelational of flow and transport over porous surfaces in a Poiseuille flow system by: 1) analyzing the drag reduction of a suspension flows over porous media and 2) understanding their related instability. I will introduce the very first continuum scale framework that accounts for the interplay of key parameters including the characteristics of the flow, the porous media and the geometry of a channel on the drag reduction. In the second part, I will characterize the flow-state boundary structure. The experimental analysis to understand the detailed analysis of the flow over and at the interface of various specific porous media using the pressure drop measurements and PIV (particle image velocimetry) technique will be also reviewed.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 268

Flow behavior of charged nanoparticle stabilized emulsions in a glass micromodel

Christopher Griffith; Hugh Daigle

1 UT Austin
Corresponding Author(s): cgriﬃth@utexas.edu

Nanoparticle stabilized emulsions have attracted interest for enhanced oil recovery (EOR) because of their improved stability to coalescence over emulsions stabilized with surfactants. This behavior is due to the irreversible adsorption of nanoparticles to the oil/water interface which can inhibit droplet coalescence. However, characterization of nanoparticle stabilized emulsions for EOR has been poor, and there is a need to understand the relationship between the static properties of emulsions (drop size and zeta potential) and their ﬂowing properties (e.g., whether drops remain stable as they ﬂow through pore restrictions). Therefore, the objective of this work was to visually study the ﬂowing behavior of nanoparticle stabilized emulsions – with different static properties - using a glass micromodel.

Nanoparticles modiﬁed with the hydrophilic silane (3-Glycidyloxypropyl)trimethoxysilane (glymo) were used to stabilize bromohexadecane-in-water emulsions. We selected glymo as a surface modiﬁer because of its demonstrated ability to sterically stabilize nanoparticles while in the presence of API brine at 80 °C. The static properties of our emulsions were altered by using different concentrations of glymo in our reaction mixtures or by varying the salt concentration in the brine. We visually monitored the ﬂowing behavior of the emulsions using 2-dimensional glass micromodel. The micromodel consists of a single 200 µm channel that reduces to a 50 µm pore restriction. We characterized the build-up and collapse of the ﬂowing emulsions at the pore restriction.

Our results suggest differences in the ﬂowing behavior of emulsions with different static properties (high vs. low zeta potential). We show that emulsions with a high zeta potential (∼18-30 mV) have a strong tendency to block the 50 µm pore restriction whereas those with a low zeta potential (∼0-5 mV) have much less of a tendency to block and build-up at the restriction. Between the two, there was a reduction in the column build-up height by a factor of 3.4. This different qualitative behavior has implications for the intended use of emulsions for enhanced oil recovery.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 354

Flow ﬁeld measurements of trapped and mobilised non-wetting phase in a microﬂuidic porous medium

Ioannis Zarikos1; Alexandros Terzis2; S. Majid Hassanizadeh1; Bernhard Weigand2

1 Utrecht University
2 Institute of Aerospace Thermodynamics (ITLR), Pfaenwaldring 31, University of Stuttgart, 70569 Stuttgart, Germany

Corresponding Author(s): i.zarikos@uu.nl

Abstract

Immiscible two-phase ﬂow in porous media is a process encountered in various applications such as oil recovery, soil remediation, CO2 sequestration and some other industrial systems. Almost all models of two-phase ﬂow are based on Darcy law, which is valid only for the phases that form a continuous domain. But, there exist many applications where one of the ﬂuid phases is (partially) discontinuous. Movement of a discontinuous phase has been the subject of various studies 1–4

There exist theories formulated on the basis of data, which analyse the phenomenon based on the overall movement of the ganglia. There is still lack of understanding of the mechanisms that lead to ganglion mobilization. One such mechanism is the interaction between the ﬂowing wetting phase and the discontinuous phase.

In this work, we focus on the interaction between the two phases and more speciﬁcally on the momentum transfer from the continuous wetting phase to the discontinuous non-wetting phase in a porous medium. As the porous medium, we used a PDMS micro-model. The non-wetting phase was doped with Rhodamine 6G particles. In this study, the setup of a La Vision MicroPIV system with
an AxioObserver.Z1 microscope was used. During the whole experimental procedure, the evolution of trapped non-wetting phases was recorded and the local velocity distributions were evaluated with Particle Tracking Velocimetry (PTV) algorithms implemented in MATLAB5. More specifically, we focus on the velocity field evolution within the ganglion and around it prior, during, and after the ganglion mobilization.

In this study, our objective is to fill this gap evaluating the steady and instantaneous flow fields inside individual droplets, blobs and ganglia using micro-Particle Image Velocimetry. Our aim is to provide a clear interpretation of how the interaction between the wetting and the non-wetting phases leads to mobilisation of the trapped phase, as the capillary number increases. Therefore, experiments are carried out prior and during the mobilisation identifying quasi-static and dynamic removal of the entrapped phases.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-G / 101

Flow of Yield Stress and Carreau fluids through Rough-Walled Rock Fractures and Packed Beads: prediction and experiments

Antonio Rodríguez de Castro¹; Giovanni Radilla¹

¹ Arts et Métiers ParisTech

Corresponding Author(s): antonio.rodriguezdecastro@ensam.eu

Many natural phenomena in geophysics and hydrogeology involve the flow of non-Newtonian fluids through natural rough-walled fractures and unconsolidated granular porous media. Therefore, there is considerable interest in predicting the pressure drop generated by complex flow in these media under a given set of boundary conditions. However, this task is markedly more challenging than the Newtonian case given the coupling of geometrical and rheological parameters in the flow law. Indeed, although recent advances have been made, obtaining a macroscopic law to predict pressure drop as a function of flow rate has proved to be a stumbling-block. In particular, extending Darcy’s and Forchheimer’s laws to the case of non-Newtonian fluids flow poses a considerable challenge. The main contribution of this work is to propose a simple method to predict the flow of commonly used Carreau and yield stress fluids through fractures and packs of spherical beads. To do so, a characteristic shear rate of the flow through the porous media is rigorously defined and an expression relating the “in-situ” shear viscosity of the fluid to the bulk shear viscosity parameters is subsequently obtained. Then, this “in-situ” viscosity is entered in the macroscopic laws to predict the flow rate-pressure gradient relations. Experiments with yield stress and Carreau fluids were
conducted using two replicas of natural fractures and 5 packs of beads and covering a wide range of injection flow rates. The results of these experiments are compared to the predictions of the proposed method, showing that the use of a constant shift parameter to relate “in-situ” and bulk shear viscosity is no longer valid in the presence of a yield stress or a plateau viscosity. This means that the relationship between characteristic shear rate in the porous medium and flow rate is not linear at low flow rates for these types of fluids. Consequently, properly representing the dependence of the shift parameter on the flow rate is crucial to obtain accurate predictions. The proposed method predicts the pressure drop in rough-walled fractures and packed beds at a given injection flow rate by only using the shear rheology of the fluid and the porosity and permeability of the medium as inputs. Our results can be included in computational studies of large-scale nonlinear flow in fractured rocks and unconsolidated granular media, which should result in improved predictions providing valuable information for management and decision making.

References:


Click here to agree

Parallel 8-B / 265

Flow patterns and rheology of confined granular media during fluid injection

Fredrik Kvalheim Eriksen1 ; Renaud Toussaint2 ; Knut Jørgen Måley3 ; Antoine L. Turquet4 ; Eirik Grude Flekkøy5

1 Porous Media Laboratory
2 CNRS, IPGS UMR 7516, University of Strasbourg
3 PoreLab, Department of Physics, University of Oslo
4 ENS Lyon
5 Corresponding Author(s): f.k.eriksen@fys.uio.no

We characterize the deformations of a dry granular medium confined inside a horizontal Hele-Shaw cell where air is injected at a constant overpressure. The overpressure is systematically varied, and we show a range of flow regimes where for example the injected fluid form channel structures similar to viscous fingers in a porous medium. By combining experimental deformation data and numerical simulations of the pore fluid pressure in the same system, we are able to analyze the rheology of the granular medium, and show that it follows a behavior similar to a yield-stress fluid. This behavior could explain the formation process of the dendritic patterns of channels empty of beads, which produces patterns in the universality class of the Dielectric Breakdown Model to the power of 2 (fractal dimensions from 1.5 to 1.6). Further, in the jammed state of the medium, we observe a stick-slip behavior where a localized region of beads suddenly rearrange and compacts, such that we have a compaction pulse moving against the pore fluid flow direction. We characterize this pulse with high speed optical imaging and acoustic measurements.

References:

Acceptance of Terms and Conditions:

Click here to agree
Poster 2 / 684

Fluid Flow Property Estimation Using a Pore Network Modeling Approach

Author(s): Edgar G. Martínez-Mendoza

Co-author(s): Martin A. Díaz-Viera ; Ana T. Mendoza-Rosas

1 Universidad Nacional Autónoma de México
2 Instituto Mexicano del Petróleo
3 CONACYT-Centro de Ingeniería y Desarrollo Industrial

Corresponding Author(s): edgar.g.martinez@hotmail.com

Pore network modeling is a technique that has been booming in recent years, and several authors
have used it to obtain properties as absolute permeability, relative permeabilities and capillary
pressures, which are common obtained from laboratory tests and/or experimental correlations. The
scope of this work is to model flow and immiscible displacement and estimate fluid flow properties
such as, absolute permeability and capillary pressure curve, using a systematic methodology.
With this in mind, the workflow begins choosing an open access carbonate’s micro-CT image and
its extracted network. The digital sample is similar to a rock sample used in a primary drainage test.
From the available information, a statistical analysis to explore the network’s topological properties
and the medium’s geometric properties is performed. This analysis will allow us to identify and
propose spatial dependencies between some properties of the network elements. Then, through mul-
tiple realizations, equivalent networks are generated using OpenPNM, an open source pore-network
modeling project. Subsequently, to simulate flow and primary drainage same conditions as those
of the laboratory test are taken into account. The Hagen-Poiseuille model and invasion percola-
tion with trapping are considered, for flow and primary drainage respectively. In primary drainage
process, statistically equivalent pore network realizations give rise to a family of capillary pressure
curves that comprises a reliability window, i.e. a value range that capillary pressure can take for the
medium under study. Finally, a capillary pressure model is fitted and the confidence intervals are
validated.

This methodology is validated in a case of study for pore network modeling of a carbonate rock
sample.

References:
neering, 18(4), 60-74. http://doi.org/10.1109/MCSE.2016.49
[Retrieved: 11-30-2017].
properties in petroleum reservoirs. (Bachelor thesis). Faculty of Engineering, Universidad Nacional
Autónoma de México. Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-H / 334

Fluid-solid reaction in single and multiphase flows by geo-material microfluidics

Joaquin Jimenez-Martinez ; Mark L. Porter ; J. William Carey ; Jeffrey D. Hyman ; George Guthrie ; Hari
Viswanathan

1 EAWAG-ETHZ
2 Bureau of Reclamation
Corresponding Author(s): jjimenez@ethz.ch

We are missing a deep understanding of the coupling of multiphase flows and fluid-solid reactions, including rock dissolution and mineral precipitation. To achieve this objective, we designed a geo-material microfluidic cell using limestone from SACROC unit (Texas, US) as substrate. For the single flow experiment, supercritical (sc) CO₂ dissolved in brine was flowed through a controlled etched geometry. In the same geometry, CO₂-saturated brine and scCO₂ were simultaneously injected for the multiphase flow experiment. Dissolution and precipitation rates for single and multiphase flows were deduced from high-precision 3D measurements, and changes in permeability from pressure measurements. We also simulated the flow through the pore space to quantify changes in flow dynamics due changes in geometry. We showed the coupling of single and multiphase flow and fluid-solid reactions, demonstrating the impact of multiphase flows on the latter.

References:

Acceptance of Terms and Conditions:
Click here to agree

POSTER 3 / 888

Forced wetting transition and bubble pinch-off in a capillary tube

Author(s): Amir Pahlavan¹
Co-author(s): Benzong Zhao ² ; Luis Cueto-Felgueroso ³ ; Gareth McKinley ¹ ; Ruben Juanes ¹

¹ MIT
² U. Toronto
³ Technical University of Madrid, Madrid, Spain

Corresponding Author(s): pahlavan@mit.edu

In their seminal works, Taylor and Bretherton showed that when a wetting viscous liquid is displaced by a less viscous non-wetting fluid in a capillary tube, a film of the defending liquid is left on the walls. Here, we revisit this classic problem in the partial wetting regime using both experiments and theory, and show that the flow dynamics drastically changes from the classic picture. We show that at a critical displacement rate a wetting transition occurs; before transition, the interface moves as a traveling wave, but beyond transition a film of the defending liquid becomes entrained on the walls of the tube. This film is unstable and recedes from the wall, forming a growing dewetting rim, which ultimately leads to bubble pinch-off. Therefore, we show that contact line dynamics can lead to macroscopic changes in the flow behavior as well as bubble/drop generation even in the absence of any geometric constraints.

References:

Acceptance of Terms and Conditions:
Click here to agree

PARALLEL 2-F / 176

Forecasting Oil Production and Economics of a Foam Pilot Including Quantitative Uncertainty Assessment

Author(s): Simon Ayache¹
Co-author(s): Frédéric Douarche ¹ ; Bernard Bourbiaux ¹ ; Frédéric Roggero ¹

¹ IFP Energies nouvelles

Corresponding Author(s): simon.ayache@ifpen.fr

This paper investigates through reservoir simulations the set-up of a foam EOR process in a real sector of a low permeability reservoir produced by waterflooding. The objectives are: to demonstrate our capability to simulate foam injection at field scale; to investigate the technical feasibility of foam injection in terms of injectivity, foam stability and improved oil recovery; and to analyze its economic feasibility as a function of technical uncertainties and market prices variations.

The study is conducted using a reservoir simulator combined with uncertainty and optimization capabilities. Our foam model modifies the gas relative permeability according to a multi-parameter mobility reduction function. Several sensitivity analyses and optimizations were performed to design the injection sequence that optimizes the foam displacement and the resulting sweep efficiency, and to determine the influence on the oil recovery and the net present value of the foam quality, its maximum gas mobility reduction, its stability and the surfactant adsorption. By applying Monte-Carlo methods on surface responses, the process robustness against surfactant adsorption and hydrocarbon prices uncertainties was assessed.

The optimization of foam injection at pilot scale requires a specific study because that process is driven by many parameters with opposite effects. Specifically we found that foam viscosity may hinder injectivity, potentially leading to a decrease in the oil production, while foam may greatly enhance displacement profiles at the same time. Moreover numerical simulations show that early gas breakthrough can occur even for highly viscous foams because the apparent foam viscosity decreases in the near wellbore due to higher velocities. This can be mitigated by performing a 3-4 months surfactant water injection pre-flush. It is then possible to find an optimal foam injection sequence that generates a high financial profit for realistic foam parameters. The foam quality turns out to be a key parameter to control the foam EOR process, with quite different values found to maximize either oil production or net present value. For the case under consideration that involves a surfactant adsorption of 250 µg/g and an optimized 5-year injection of a foam of quality 0.45 following a surfactant aqueous pre-flush, we show that the foam process is profitable and robust with respect to market prices variations and technical uncertainties.

This innovative optimization methodology shows that foam processes could be eligible for this pilot. After designing properly the injection sequence, including a surfactant pre-flush prior to foam injection, reservoir simulations predict that this EOR process may highly improve the exploitation profitability. Moreover profitability is robust to economic uncertainties, with a breakeven price of 30 $ per barrel, as well as technical uncertainties, of which adsorption up to 600 µg/g.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 788

FraC: a DFN conforming meshing approach used to obtain reference simulations for steady-state flow, transport and well-test simulations

Tri Dat Ngo¹ ; André Fournoi ; Benoit Noetinger¹

¹ IFPEN

Corresponding Author(s): andre.fourno@ifp.fr

Although modeling transfers through naturally fractured media has been the subject of extensive investigation since the 1960’s (Bear et al. 1993, Berkowitz 2002, Adler et al. 2012), it remains a
challenging field of research. Applications range between management of polluted groundwater, nuclear waste storage (Fournou et al. 2004), CO2 sequestration (Verscheure et al., 2012), oil field production or geothermal energy, this challenge have to be addressed. Numerous approaches have been proposed and may be divided into two sets: i) the continuous approaches (Fournou et al., 2013) where fractures are taken into account via equivalent properties and ii) the discrete approaches where each fracture with explicit geometry is modeled within a complex discrete fracture network (DFN) (Khvoenkov and Delorme, 2011; Noetinger and Jarrige, 2011). This work focuses only on discrete models.

The main difficulty of discrete methods is to build high-quality meshes for complex DFN geometries. The cornerstone of our Fracture Cut approach (FraC) is to decompose each fracture into a number of connected closed contours in which fractures intersections are located on their boundaries. The contour boundaries shared between intersecting fractures are then discretized in a conform manner. The resulting conforming meshes closely respect the DFN geometry; even tiny fractures are taken into account to conserve the DFN connectivity. Furthermore, flexible strategies for moving or adding intersecting points are applied to ensure a good quality of the final mesh. The shortcoming of this approach is that it increases the number of fracture intersection tests and consequently the execution time. Advanced techniques like local mesh refinement or parallel computing are applied to improve the computing performance.

The FraC approach has already been tested and validated for simulating steady-state flow and transport processes (Ngo et al., 2017). The objective of this contribution is to present some new results for well-test simulations run on FraC’s meshes. For this purpose, the complex fracture network from the synthetic Bloemendaal reservoir will be employed. The Bloemendaal field is a 12 × 15 km oil saturated carbonate reservoir that consists in a North/South oriented anticline structure characterized by 3 units, 3 rock types and 3 diffuse fracture sets. Bloemendaal reservoir faults are also known to be transversal barriers for fluids. In addition these faults are suspected of being longitudinal drains, which can be modeled using fault-related fractures. Our preliminary results emphasize the effect of these faults on well-test analysis.

References:
Click here to agree

Poster 1 / 55

Fractal model of gas diffusion coefficient through porous nanofibers with rough surfaces

qian zheng\textsuperscript{None}; jintu fan\textsuperscript{None}; xiangpeng li\textsuperscript{None}; shifang wang\textsuperscript{None}

Corresponding Author(s): thbfbzhengqian@163.com
Fractal model of gas diffusion coefficient is derived for porous nanofibers, which are assumed to be composed of a bundle of tortuous capillaries whose pore size distribution and roughness of wall surfaces of capillaries follow the fractal scaling laws. The analytical expression for gas relative diffusion coefficient is a function of the relative roughness, fiber radius and microstructural parameters (porosity, the fractal dimension for pore size distribution and tortuosity, the maximum and minimum pore diameter and the characteristic length). The proposed fractal model is validated by comparison with available experimental data and correlations. At the same time, the effect of microstructural parameters of porous nanofibers on gas diffusion has been studied in detail. The results show that roughness of wall surfaces of capillaries in porous nanofibers should not be neglected. It is believed that the current work can reveal gas diffusion mechanism in porous nanofibers and may be applied in other porous materials.

References:

Parallel 3-D / 534

**From Images to Rock Properties**

Arash Aghaei¹; Connor Burt¹; Gwenole Tallec¹

¹ Thermo Fisher Scientific

Corresponding Author(s): arash.aghaei@fei.com

From Images to Rock Properties
In the Oil and Gas industry, digital images of rock samples are being collected and utilized for reservoir formation characterization more frequently than ever. This is in part due to the fact that imaging tools such as X-ray CT scanners and SEM’s have become more prevalent, and also due to the challenges and time-consuming processes in traditional core analysis of unconventional and complicated conventional reservoirs. Rock images (e.g. optical images of thin section) have traditionally been used for qualitative and to a limited extent quantitative analysis of rocks, often using laborious point-counting methods. With the advent of computerized image analysis techniques and image-based simulation models, the information that can be obtained from rock images has been tremendously improved both in quantity and quality. Nowadays, one can use rock images to characterize the pore-space of a rock sample to calculate porosity and then simulate the fluid flow in the digitally characterized pore-space to calculate permeability and even multi-phase flow properties. The accuracy of the image-based results would depend on the quality of the images, the resolution at which the images are acquired, and the algorithms behind the image analysis and image-based modeling tools. Having high-quality imagery data at multiple scales and multiple resolutions, and consistent and robust image analysis workflows is the key for achieving the best results. PerGeos, the Digital Rock Image Analysis and Modeling Suite has been developed for large and multi-modal data analysis. Using this software suite, one can analyze data from multiple sources and at multiple scales. Combined with the workflow automation capability, the analysis tools in PerGeos are used to generate effective workflows for various types of data and analyses. An overview of the digital rock technology will be presented in this talk. Examples of micro-CT, whole core CT, SEM, and FIB-SEM data analysis of rock samples will be shown.

References:

Parallel 9-G / 728
From Pore to Porous Media: A Connected Hierarchy of Chaos

Guy Metcalfe¹ ; Daniel Lester² ; Mike Trefry³

¹ Monash University
² RMIT University Melbourne
³ independent researcher

Corresponding Author(s): guy.metcalfe@monash.edu

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-B / 511

From Red Cells to Soft Porous Lubrication

Qianhong Wu¹ ; Zenghao Zhu²None ; Rungun Nathan²

¹ Villanova University
² Penn State Berks

Corresponding Author(s): qianhong.wu@villanova.edu

In this paper, we report a novel experimental study to examine the lubrication theory for highly compressible porous media (Feng & Weinbaum, JFM, 422, 282, 2000), which was applied to the frictionless motion of red cells over the endothelial surface layer (ESL). The experimental setup consists of a running conveyor belt covered with a soft porous sheet, and an upper planar board, i.e. planing surface. The pore pressure generation was captured when the planing surface glides over the porous sheet. If the lateral leakage was eliminated, we found that the overall pore pressure’s contribution to the total lift, $f_{\text{air}} \times 80\%$, and the friction coefficient $= 0.00981$, when $U = 5 \text{ m/s}$, $L = 0.381 \text{ m}$, $= h_2/h_0 = 1$ and $k = h_2/h_1 = 3$, where $U$ is the relative velocity of the conveyor belt; $L$ is the length of the planing surface; $h_0$, $h_1$ and $h_2$ are the undeformed, leading edge and trailing edge porous layer thickness, respectively. $f_{\text{air}}$ increases with the increase in $U$, and $L$, while decreases with the increase in $k$. decreases with the increase in $f_{\text{air}}$. If later pressure leakage exists, the pore pressure generation is reduced by nearly 90%. All the experimental results agreed well with the theoretical predictions. The study presented herein lays the foundation for applying soft porous media for new type of bearing with significantly reduced friction.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-C / 710

Fully-coupled Geomechanics and Flow with Embedded Meshes

Rami Younis¹ ; Guotong Ren¹

¹
Corresponding Author(s):

Geomechanical effects can have a first-order effect on production from naturally and hydraulically fractured reservoirs. Unstructured discrete fracture-matrix methods utilize conforming meshes with fractures represented by N-1 dimensional elements with local mesh refinement about them. Numerous coupled mechanics and flow models are employed on such mesh topologies. While these methods can offer attractive properties in terms of accuracy, they do rely on the availability powerful mesh generators. Moreover, their application to fracture propagation modeling requires mesh adaptivity. Embedded mesh methods on the other hand aim to couple independently constructed meshes for the matrix and fractures without the need for the meshes to conform. One timely challenge is the design of accurate and efficient numerical schemes for coupled mechanics and multiphase flow. In this work, a hybrid discretization is proposed; pEDFM (projection-based embedded discrete fracture) is adopted for multiphase flow and is fully-coupled (monolithic) to an extended finite element method (XFEM) for geomechanics. Three aspects of the scheme are analyzed: accuracy, nonlinear solvability, and the efficacy of linear preconditioners for the resulting linearized residual systems. The grid refinement is performed to test the convergence rates for different physical variables (pressure, saturation and displacement). We use the block LDU factorization so that two different AMG (algebraic multigrid method) for XFEM and EDFM can be applied separately. AMG will be called whenever it is required by the outer loop solver, FGMRES.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 1122

Fundamental study of water evaporation in cold asphalt mixture

Author(s): Tahseen Saadoon

Co-author(s): Alvaro Garcia ; Breixo Gomez Meijsde

Corresponding Author(s): evxtds@nottingham.ac.uk, ezzag2@exmail.nottingham.ac.uk, ezzbg@exmail.nottingham.ac.uk

Cold asphalt mixture (CAM) is a road materials obtained by mixing bitumen emulsion, aggregate, water and often cement at ambient temperature. When using CAM, aggregates and binder do not need to be heated during the mixing operation, which brings social, economic and environmental benefits compared to other paving materials, such as hot mix asphalt (HMA).

Like other types of asphalt materials, CAM require manufacturing operations, such as mixing, storage, laying and compaction during production, but additionally, they also need a curing stage. This fundamentally important stage, involves the evaporation of water/volatiles from the mix and the beginning of setting, which results in increased bonding among bitumen particles and between these and the other materials in the mix. Its development determines the need to open the road to traffic and the mechanical properties during service life.

In CAM, high portion of water remains trapped inside their structure, taking long time to evaporate completely and producing poor mechanical performance during the first stages of road service life. This problem is particularly highlighted in areas with cold and wet climate conditions. Therefore, CAM have been generally restricted to the construction of the non-structural pavement layers.

For this reasons, and in order to underpin the use of CAM, the evaporation of interstitial water must be accelerated and optimised. Since the pioneering uses of CAM to the present, many studies have aimed to improve the curing of CAM through different techniques, such as the addition of cement. Despite these attempts, CAM still presents slow mechanical development in comparison to main competitors (e.g. HMA).

This research aims to understand the dynamics of water evaporation in CAM, with without and cement additions and compare them to soil/granular unbound materials (without binder). With this purpose, dynamic water evaporation and hydraulic conductivity tests were carried out. Moreover,
the pore size distribution index (n) for the different samples and its evolution over the drying time were estimated based on hydraulic conductivity tests. These results showed the relationship between the internal pore distribution and water dynamics during drying. In addition, it was seen that bitumen emulsion is the main component that delays the curing process of cold mix asphalt and the type and quantity of cement used in this research did not significantly help to accelerate it.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-C / 1118

GENFIELD: a parallel software for the generation of stationary Gaussian random fields

Geraldine Pichot¹; Simon Legrand¹; Jocelyne Erhel¹; Mestapha Oumouni²

¹ Inria
² Université de Nantes

Corresponding Author(s): simon.legrand@inria.fr

In this work, we present a parallel MPI software, called GENFIELD, to generate stationary Gaussian random fields, based on the circulant embedding method [7, 1, 4]. The advantage of the circulant embedding method over existing methods (Cholesky factorization of the covariance matrix, Karhunen Loève series expansion) is its computational efficiency. It relies on Discrete Fourier Transform that can be computed efficiently with a Fast Fourier Transform algorithm. In GENFIELD, we use the FFTW3 library [8], which performs MPI parallel one-dimensional transforms. To ensure reproducibility and independence between the generated fields, we take benefit of the streams and substreams structure offered by the Ringstream library [5].

GENFIELD is used in hydrogeology to model natural fields, like hydraulic conductivity or porosity fields [3, 6]. Such fields are a pre-requisite for uncertainty quantification studies [2].

References:


References:

Acceptance of Terms and Conditions:
Click here to agree
Poster 4 / 476

GP-GPU for DFN flow simulations

Stefano Berrone$^1$; Alessandro D’Auria$^2$; Sandra Pieraccini$^2$; Stefano Scialò$^2$; Fabio Vicini$^2$

$^1$ Politecnico di Torino, Italy
$^2$ Politecnico di Torino

Corresponding Author(s): fabio.vicini@polito.it

The present work proposes the use of General-Purpose Graphics Processing Units (GP-GPUs) to solve flow problems in large scale Discrete Fracture Networks (DFNs). Discrete fracture networks are randomly generated sets of planar polygons in the three dimensional space resembling the fractures in the subsoil. Recently a minimization approach was developed to tackle the issue of effective flow simulations in intricate networks of fractures [1,2,3,4]. If the minimization problem is solved via a gradient based approach, the computation of the descent direction at each iteration requires several matrix-vector operations that involve quantities related to each fracture in the network and that can be performed in parallel. Thus, the use of GPUs appears very promising to accelerate computations. In this context, one of the principal bottlenecks consists in the communications between the GPU and the main-board through the bus PCI-Express. The code is organized in a way that minimizes these communications, allowing, at the same time to optimize the use of all cores in the graphic unit when performing floating-points operations. The code has been developed for GPUs with CUDA (NVIDIA) architecture using the cuSparse and cuBlas libraries to handle operations on both sparse and dense matrices. Experiments show that maximum speed-ups are mainly affected by the number of intersections in the considered DFNS with speed-ups approaching 20x in networks with a large number of intersections.

References:


Click here to agree

Poster 4 / 273

Gas flow through corroded wellbore casing

Ishtiaque Anwar$^1$; Mahya Hatambeigi$^2$; Mahmoud Reda Taha$^2$; John Stormont$^1$

$^1$ University of New Mexico
$^2$ The University of New Mexico

Corresponding Author(s): ishti@unm.edu

References:

Acceptance of Terms and Conditions:

Click here to agree

Page 215
Parallel 9-A / 25

**Gas transport in porous geological media with contract of properties, and irregular distribution of pores.**

Viktoria Savatorova\(^1\); Aleksei Talonov\(^2\)

\(^1\) **UNLV**  
\(^2\) **MEPhI**

**Corresponding Author(s):** viktoria.savatorova@unlv.edu

In this work, we perform multiscale modeling of gas transport through the heterogeneous solid having irregular pore structure and contrast of properties on different spatial scales. We assume that the solid consists of inorganic material (clay, sand) with organic (kegogen) inclusions imbedded into it. There exist a contrast of properties and spatial scales between the matrix and inclusions. The pore sizes vary from micro to nanometers, permeability and diffusivity can differ by several orders of magnitude. We consider filtration and molecular diffusion as mechanisms for the free gas transport, and surface diffusion as a main mechanism of gas transport through nanoporous organic inclusions. The irregularities of porous structure we characterize by their deviations from the regular (periodic) distribution.

Multiscale analysis is applied to mass balance equations, the equation of state for free gas, and an isotherm of adsorption. We focus on the upscaling from pore-scale to the core-scale and then from core-scale to reservoir scale.

As a result of upscaling, we get a macroscopic equation describing gas transport through an effective medium. It turns out that macroscale parameters characterizing gas transport depend on diffusivity, permeability, and porosity of components of the system, the amount of inclusions and their spatial distribution. We investigate sensitivity of macroscale parameters to deviations in pore distributions from their averaged values. We also determine the distribution of gas concentration through the production time and evaluate the production rate as a function of time.

**References:**


Click here to agree

---

Parallel 6-E / 697

**Gassmann Equation for Nanoporous Media**

Gennady Gor\(^1\); Boris Gurevich\(^2\)

\(^1\) **New Jersey Institute of Technology**  
\(^2\) **Curtin University**

**Corresponding Author(s):** gor@njit.edu

Recent progress in extraction of unconventional hydrocarbon resources, in particular shale gas, has ignited the interest in the studies of fluid-saturated nanoporous media. Since many thermodynamic and mechanical properties of nanoscale solids and fluids differ from the analogous bulk materials, it is not obvious whether wave propagation in nanoporous media can be described using the same framework as in macroporous one. Prior to approaching media as complex as shales, it is necessary to get a thorough understanding of wave propagation in simpler nanoporous media, e.g. a widely studied Vycor glass.

Here we test the validity of classical Gassmann theory of wave propagations in saturated media. We consider the literature data on longitudinal and shear ultrasonic velocities in nanoporous Vycor
glass as a function of pressure of n-hexane and argon vapors respectively [2,3]. The quantitative testing of the Gassmann theory on Vycor glass requires the knowledge of the bulk modulus of the solid nonporous glass $K_S$, which is impossible to measure directly. We propose to estimate $K_S$ from the so-called pore-load modulus obtained from measurements of the adsorption-induced deformation [4]. Furthermore, comparison of this estimate with the estimates from the elastic effective medium theory gives a recipe for estimating $K_S$ when adsorption-induced deformation data are not available. The fluid modulus can be calculated according to Tait-Murnaghan equation at the solvation pressure in the pore [5]. Substitution of these parameters into Gassmann equation provides predictions consistent with measured data. Our findings set up a theoretical framework for investigation of fluid-saturated nanoporous media using ultrasound [6].

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-H / 188

Harnessing highly non-linear structures for amplified attenuation by local flow

Patrick Kurzeja

1 Institute of Mechanics, TU Dortmund, Germany

Corresponding Author(s): patrick.kurzeja@tu-dortmund.de

Highly non-linear, porous structures stand out by significant changes of their morphology, allowing to control, e.g., their size, shape and acoustic band gaps. A research area that still remains to be fully explored in this exciting class of functional materials is their interaction with pore fluids. For example, the local-flow phenomenon is well studied for rocks, describing a local exchange of pore fluid between adjacent cavities [1,3]. While local flow constitutes the major attenuation mechanism for fluid-filled rocks, it lacks attention for non-linear structures. We present the influence of non-linear structural deformations on the local-flow mechanism, aiming at the potential of high attenuation at low frequencies. The use of non-linear structures allows to amplify or even trigger local flow [2]. Structures prone to local flow will be discussed and the most efficient geometries will be highlighted in terms of low-frequency attenuation.

References:


Click here to agree

Parallel 11-B / 877

Heating by underground ice storage

Jacco Haasnoot

David Smulders

Wijnand Heems

Eindhoven University

Corresponding Author(s): haasnoot@cruxbv.nl

One of the key factors in energy transition is energy storage. As most of the energy in the Netherlands is used for heating, the focus on renewable energy sources is on capturing and using heat in an effective way. We have developed a system for underground heat storage that is based on ground freezing principles (also called ice storage). It is based on the fact that the phase change enthalpy of water from liquid to solid can be used for energy storage. During the freezing process of one kg of water, 333 kJ (0.093 kWh) is released. Hence, if a certain amount of groundwater can be frozen or heated up with a heat pump, energy can be stored and extracted. We discuss the experimental set-up to validate the storage principle and we compare the experimental results with numerical predictions.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 20

Hierarchically porous hydroxyapatite ceramics prepared with wheat flour and their microstructural characterization via mercury porosimetry, image analysis and tomography

Eva Gregorová

Tereza Uhlírová

Petra Diblíková

Anastasia Brinjeva

Willi Pabst

University of Chemistry and Technology, Prague

UCT Prague

Corresponding Author(s): eva.gregorova@vscht.cz

Hydroxyapatite (HA) is the main inorganic component of human bone and therefore HA ceramics are widely used as artificial replacements for natural biomaterials, both for implant applications and bone tissue engineering scaffolds [1-3]. In order to ensure not only biocompatibility (bioactivity), but also osteoconductive and osteoinductive properties enabling bone cell ingrowth, as well as sufficient delivery of nutrients, drugs and/or growth factors, the microstructure of these artificial biomaterials has to be hierarchically porous, i.e. similar to the microstructures of natural cortical or trabecular bone. In the present work hierarchically porous HA ceramics, i.e. ceramics with a wide range of pore sizes, has been prepared by a new ceramic shaping and foaming technique using starch and wheat flour [4,5]. Aqueous HA suspensions have been prepared with commercially available HA powder (tribasic calcium phosphate with 30–40% Ca, Alfa Aesar, Germany) in concentration 36 wt.% with 0.7 wt.% dispersant (Dolapix CE64, Zschimmer & Schwarz, Germany), 20 vol.% wheat flour and 5 vol.% corn starch. The wheat flour acts as a foaming agent (foaming being achieved by ball milling in polyethylene bottles with alumina balls for 6 h), while the corn starch
acts as a foam stabilizer (stabilization being achieved via starch gelatinization during heating at 80 °C for 6 h), improves dimensional accuracy and increases the strength of the materials before firing. After drying (105 °C) the samples were fired to 850 and 1200 °C (heating rate 2°C/min, dwell time 2 h) and characterized by X-ray diffraction, where HA has been confirmed as the only phase in both cases. Mercury porosimetry confirmed open porosities of 83 and 66 % as well as trimodal and bimodal pore size distributions after firing at 850 and 1200 °C, respectively (with modes at around 100 µm and 1 µm in both cases and an additional pore size mode below 100 nm for the material sintered at 850 °C). Based on scanning electron microscopic images of polished sections of samples immersed in and infiltrated with transparent epoxy resin (Araldite 2020, Ciba, Germany), the complete set of global microstructural descriptors has been determined via image analysis (porosity, surface density / mean chord length and mean curvature integral density / generalized Jeffries size) [6,7]. Additionally, based on spatial images obtained via X-ray microtomography, the total curvature integral density / 3D Euler characteristic has been determined. Finally, size distributions of the large pores (i.e. the foam bubbles representing approximately 50 ± 2 % porosity in both cases) have been determined, corrected for the random section problem [8], transformed to volume-weighted distributions and compared to the pore size distribution determined directly from tomography (using the Hildebrand-Rüegsegger thickness measure) and the pore throat size distributions determined via mercury porosimetry.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 56

High order methods for the simulation of viscous fingering

Author(s): Beatrice Riviere*
Co-author(s): Jizhou Li

Corresponding Author(s): riviere@rice.edu

A high order method is formulated for solving the miscible displacement problem and modeling viscous fingering. Viscous fingering in porous media may occur when a fluid with low viscosity is used to displace a fluid with high viscosity. For this type of flow instability, a tiny perturbation can be amplified exponentially, which triggers a finger-like pattern in the fluid concentration profile during
the fluid displacement. The miscible displacement problem consists of a coupled system of differential equations with primary unknowns pressure and concentration of the injected fluid. The numerical method is based on the discontinuous Galerkin method with weighted average stabilization technique and flux-reconstruction post-processing. Simulations in two and in three dimensions show the growth and propagation of fingers for large mobility ratios and large Peclet numbers. Results are compared with those obtained by using a generic cell-centered finite volume method. Finally we show some scalability results for a three-dimensional core flooding.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 6-H / 152

High performance SPH implementations for pore scale direct numerical simulations

Author(s): Maria Osorno

Co-author(s): Malte Schirwon \(^1\); Nadine Falkner \(^1\); Rakulan Sivanesapillai \(^1\); Dominik Göddeke \(^1\); Holger Steeb

\(^1\) University of Stuttgart

Corresponding Author(s): maria.osorno@mechbau.uni-stuttgart.de

The study of fluid-flow through porous materials is of high relevance in a wide variety of applications such as geothermal energy exploration and generation, CO2 sequestration and oil and gas reservoirs management. Physical experiments are not always convenient or even feasible, due to the nature of the materials. A suitable alternative is to realize Direct Numerical Simulations with micro-CT characterized porous materials geometries.

Often, the microstructure of porous media presents a very complex geometry. Moreover a complete study of fluid-flow through porous media, require simulations in a wide range of Reynolds numbers. The Smoothed Particle Hydrodynamics (SPH) method fits clearly to the desired applications. SPH is a meshless Lagrangian method; its meshless nature simplify the treatment of complex geometries because particles can be directly linked to the voxels, avoiding pre-processing steps for mesh-generation. Furthermore, the Lagrangian framework, facilitate the simulation of fluid-flows at high Reynolds numbers because non-linear convection terms do not need to be specifically treated. However, SPH as a particle technique requires high computational resources, especially for simulations of large domains.

To overcome these difficulties, we have extended the highly optimized HOOMD-blue to include the SPH method for quasi-incompressible single phase and two-phase fluid flow. HOOMD-Blue is a general purpose particles simulation tool-kit initially developed for molecular dynamics. The software was implemented for GPU parallelization and later on, MPI domain decomposition was included. Our SPH module targets both CPUs and GPUs.

We present initial scalability studies of the SPH module for quasi-incompressible single phase flow for a variety of representative test cases. The simulations are performed on the supercomputers Hazel Hen (HLRS – Germany) and Piz Daint (CSCS – Switzerland) for the CPU and GPU parallelization respectively.

We present additionally simulations of fluid flow in a large-scale high-resolution imaged real porous material at different Reynolds numbers, and estimate different effective transport properties of the material, such as permeability and tortuosity. We compare the computed effective properties, with the ones estimated with other more classical grid-based numerical methods.
Future work includes the implementation of additional models such as solid-solid and deformable solid-fluid interaction. Furthermore, we are aiming to improve the present SPH module with additional time integration methods.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 936

High-Resolution Monitoring of Nanoparticle Transport Behavior in Multi-Phase Saturated Porous Media: Experimental Study

Author(s): Jelayne Falat¹
Co-author(s): Adam Fehr ¹ ; Ali Telmadarrieie ² ; Steven Bryant ³

¹ CERC Co-op Student
² Postdoctoral Research Fellow
³ Professor

Corresponding Author(s): steven.bryant@ucalgary.ca

Nanoparticles are emerging as an important advancement in the petroleum industry, including in enhanced oil recovery. Nanoparticles have shown potential to mitigate some of the issues associated with enhanced oil recovery due to their impact on bulk and interfacial properties. However, before their application in any EOR operation, the study of nanoparticle transport behavior in porous media is of prime importance. The reservoir condition such as high temperature, high pressure, the presence of multi-phase fluids, and salinity can significantly affect the nanoparticle transport behavior, which is the focus of this study.

In order to understand the behavior of nanoparticles in porous media, a series of single-phase and multi-phase nanofluid floods were performed through unconsolidated sandpacks under reservoir conditions. Using a highly specialized core flooding apparatus with the capacity to handle high temperature (150 °C) and high pressure (35 MPa), nanofluid slugs were injected into the porous media followed by a post-flush of brine. An inert chemical tracer was used to characterize the dispersivity of the porous media. Experimental variables included the type of nanoparticle, concentration, salinity, temperature (up to 120 °C), pressure (up to 5 Mpa), flow rate, and effect of oil (Dodecane). Propagation was observed through the sandpack using four differential pressure transducers located along the length of the pack. Measurements of permeability were taken before and after the nanofluid slug at varying flow rates in order to determine the effect of the nanoparticle on permeability. High-resolution analysis of the concentration of nanoparticles in the influent and effluent from analysis by Triple Quadrupole ICP-MS provided the breakthrough curve, as well as the adsorption and retention of the nanoparticles in the sandpack.

The result of this study indicated that the factors affecting nanoparticle transport and retention the most were nanoparticle type, salinity, and the presence of oil phase. The pressure (up to 5 Mpa) and temperature (120 °C) were shown to have an insignificant effect on the behavior of the studied nanoparticles in the porous media. According to the particle size measurement and ICPMS results, the retention of uncoated silica nanoparticles was the same in the presence of oil compared to that of single-phase retention where recovery of nanoparticle was more than 80%. The increase in the post-flush flow rate (10 times) did not increase the nanoparticle recovery. While increasing
the salinity was shown to reduce fines migration, it reduced the stability of the nanoparticles and caused aggregation, resulting in increased retention and permeability reduction. However, some of the studied nanoparticles showed good salt tolerance at reservoir condition. In addition, the studied silica nanoparticle had minimal permeability reduction, making them a viable option for additives in EOR. Furthermore, the results of multiphase flow experiments showed that the presence of fines in the porous media, and their combination with nanofluid resulted in emulsion generation and oil recovery up to 70% while the nanofluid and oil phase did not make any emulsion in bulk tests study. The results of this study broaden our understanding of how nanoparticles interact in porous media under reservoir conditions. Once the mechanisms of nanoparticle transport and retention are better understood in single-phase and multi-phase transport, they can be studied in a wide range of applications including polymer flooding, surfactant additives, and steam-foam stabilization. Nanoparticles have the potential to improve enhanced oil recovery by reducing chemical additives and water required, making existing methods more effective, and reducing the environmental impact of oil recovery processes.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 871

High-Resolution, Rock-Based, 2.5D Polymer Micromodels

Daniel Park\(^1\); J. Upadhyay\(^1\); Karsten Thompson\(^2\); Dimitris Nkitopoulos\(^2\)

\(^1\) Louisiana State University

\(^2\) Louisiana State University, Mechanical and Industrial Engineering Department

Corresponding Author(s): medimi@lsu.edu

Micromodels have been widely used to study the transport mechanism of fluids at pore-scale for subsurface engineering applications such as enhanced oil recovery. Micromodels with small feature sizes can be manufactured by lithography-based microfabrication on Si or glass, but they are in general restricted to 2D representation of pore network geometry. Recently our group demonstrated more realistic 3D representation of an actual reservoir rock-derived sample in a 2.5D polymer micromodel using micromilling of a brass mold and hot embossing of polymethylmethacrylate (PMMA). However the resolution of this micromodel was limited to 25 μm due to minimum usable milling tool size.

In this work, we present fabrication of high-resolution, rock-based, 2.5D polymer micromodels, and flow visualization in such micromodels for the investigation of fluid transport mechanisms at pore-scale. In order to improve the minimum resolution of 25 μm in the 13-layered micromodels made from the micro-computed tomography images of a Boise rock, the same pore geometries were scaled down to the resolution of 5 μm and 10 μm to demonstrate the manufacturing feasibility of high-resolution, rock-based, 2.5D micromodels. The original low-resolution micromodel was included. Additional features such as fluidic ports, the inlet and outlet regions, and fluidic distribution channels were added. The flow connectivity of pores from the inlet to the outlet was provided by the 12th and 13th layers.

Multilayer lithography of SU-8 with a target thickness of 5 μm for each layer was carried out on seed layer coated Si substrates with process optimization to obtain 13-layered SU-8 molds. After processing of the 1st SU-8 layer, flycutting-based process was tested for the next 12 layers. Flycutting method after spin-coating of thick SU-8 allowed the tight control of the overall thickness variation within ± 1.5 μm without pattern distortion even for 5 μm resolution. Electroforming of nickel was performed in SU-8 molds prepared by flycutting-based lithography process. Electroforming in the SU-8 molds revealed the high-quality pattern formation in the 13 nickel layers, thus confirming the excellent feature fidelity control down to 5 μm resolution. The nickel mold was used for hot embossing of PMMA to make high-resolution, rock-based, 2.5D polymer micromodels. The micromolded
2.5D micromodels showed significant resolution improvement by up to 5-fold from the previous 2.5D micromodels and rendered the real pore network geometry of the 3D reservoir rock.

The hot embossed 2.5D micromodels in PMMA were sealed by thermal fusion bonding and used for flow visualization. The dye-filled polymer micromodels (10 μm and 5 μm resolution) showed the flow connectivity and pore depth variations. Fluidic experiments were carried out by injecting fluorescent nanoparticles and particle transport was observed. Several preferential flow paths were similarly observed for both the 10 μm and 5 μm resolution micromodels. There were some differences in local particle accumulations over time between the two micromodels. Further characterizations to investigate the correlations of fluid flow to the pore depth variations and the pore space resolution will aid in understanding of the complicated fluid transport in the real 3D reservoir rocks.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 364

High-order space-time approximations of dynamic poroelasticity models

Uwe Koecher1; Markus Bause1

1 Helmut-Schmidt-University Hamburg

Corresponding Author(s): koecher@hsu-hamburg.de

The accurate high-order approximation in space and time is of fundamental importance for the simulation of dynamic poroelastic models which include coupled fluid flow, deformation and wave propagation.

Dynamic poroelastic models appear for example Lithium-ion battery fast-charge simulations and include sharp concentration and pressure gradients, high mechanical stresses, elastic wave propagation, memory-effects on the permeability, multi-phase behaviour and electro-chemical reactions.

In this contribution our high-order space-time discretisations, including mixed finite elements (MFEM) for the flow variables and interior-penalty discontinuous Galerkin finite elements (IPDG) for the displacement and velocity variables, are presented. For the discretisation in time we use a high-order accurate discontinuous Galerkin dG(τ) discretisation.

The arising linear block systems are solved with our sophisticated monolithic solver technology with flexible multi-step fixed-stress preconditioning. Inside the preconditioner highly optimised system solvers for low order approximations can be used. Additionally, our solver technology allows for parallel-in-time application.

The performance properties and their potential for battery simulations and further applications are illustrated by challenging numerical experiments.

References:


Parallel 3-G / 556

Higher order multipoint flux mixed finite element methods on quadrilaterals and hexahedra

Ilona Ambartsumyan1 ; Eldar Khattatov1 ; Jeonghun Lee2 ; Ivan Yotov1

1 University of Pittsburgh
2 The University of Texas at Austin

Corresponding Author(s): yotov@math.pitt.edu

We develop higher order multipoint flux mixed finite element (MFMFE) methods for solving elliptic problems on quadrilateral and hexahedral grids that reduce to cell-based pressure systems. The methods are based on a new family of mixed finite elements, which are enhanced Raviart-Thomas spaces with bubbles that are curls of specially chosen polynomials. The velocity degrees of freedom of the new spaces can be associated with the points of tensor-product Gauss-Lobatto quadrature rules, which allows for local velocity elimination and leads to a symmetric and positive definite cell-based system for the pressures. We prove optimal k-th order convergence for the velocity and pressure in their natural norms, as well as (k+1)-st order superconvergence for the pressure at the Gauss points. Moreover, local postprocessing gives a pressure that is superconvergent of order k+1 in the full L2-norm. Numerical results illustrating the validity of our theoretical results are included.

References:
Acceptance of Terms and Conditions: Click here to agree

Parallel 5-C / 239

Homogenization of a Stokes-Biot system modeling deformable fractured and vuggy porous media

Jun Yao3 ; Zhaoqin Huang2

1 Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China), Qingdao, China
2 China University of Petroleum (East China)

Corresponding Author(s): huangzhqin@upc.edu.cn

Vugs and fractures have significant impacts on the fluid flow paths through fractured and vuggy porous media. On the other hand, the presence of vugs and fractures also can significantly affect the geo-mechanical behavior of the porous media. How to quantify and analyze the accurate effects of the vugs and fractures on the hydro-mechanical behavior of the media is still an opening and challenging problem. To this end, we systematically derive a macroscopic poroelastic model for a single-phase, incompressible, viscous fluid flow in a deformable fractured and vuggy porous medium. Herein, we assume that a fractured and vuggy porous medium is divided into two parts, i.e., the porous matrix and fractures/vugs, on a mesoscopic scale (e.g. lab core scale). In the porous matrix, the classical Biot’s equations are used to model the poroelastic process. In fractures and vugs, the Stokes equations are applied to model the free fluid flow, which couple with Biot’s equations through the extended Beavers-Joseph-Saffman (BJS) boundary condition on the porous-fluid interface. Through a two-scale homogenization limit as the period tends to zero, we obtain a macroscopic
Biot’s equations governing the fractured and vuggy medium on macroscopic scale. The homogeniza-
tion approach determines the form of the macroscopic constitutive relationships between variables,
and shows how to compute the poroelastic coefficients in these relationships. It should be noted
that the calculations of the macroscopic properties only depend on the decoupling three base cell
problems, i.e., two Navier equations for elastic problem and one Darcy-Stokes flow problem with BJS
conditions. It is shown that our homogenized results provide a natural way of modeling deformable
realistic fractured and vuggy porous media.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-B / 780

Homogenization of advection-diffusion and solid diffusion in poro-
elastic media for modelling transport of soluble factors in biolog-
ical tissues

Pascale Royer¹; Pascal Swider²; Pauline Assemat²

¹ LMGC (Univ. Montpellier and CNRS)
² IMFT (Univ. Toulouse, CNRS)

Corresponding Author(s): pauline.assemat@imft.fr

This work has been motivated by the study of solid tumor growth, and more specifically, by the
examination of the most frequently encountered type of pediatric primary bone tumors (osteosar-
coma), characterised in their early stage by the formation of non-mineralised bone tissue, called osteoid [2].
As the tumor evolves in time, mineralisation of this growing tissue can take place. The
objective of this work is thus to investigate the advection-diffusion of soluble factor such as calcium
and phosphate [2] in the context of tumor mineralisation, to examine how the mineralisation of
bone tissue may become a barrier to treatment in the context of drug transport [3], and also to
determine how proteins and growth factors can play a role in tumor growth [4]. For this purpose, the
mathematical modelling of advection-diffusion and solid diffusion in a poroelastic medium is firstly
required. The present work is thus aimed at deriving the models by using asymptotic homogeniza-
tion. Macroscopic models are derived by starting from the pore-scale equations. They describe a
deforming linear elastic solid matrix saturated by a Newtonian incompressible fluid. They further
include the convection-diffusion equations in the fluid phase, with a magnitude of the Peclet number
that corresponds to a macroscopic advective-diffusive regime, and also account for diffusion in the
solid phase. The local fluid/solid equations lead to Biot’s model of poroelasticity on the macroscopic
scale. Then, homogenization of the transport equations gives rise to three possible macroscopic ac-
dective diffusive transport models, that relate to three possible orders of magnitude of the diffusivity
ratio: a model in which the solid diffusion only influences the accumulation term; ii) a model with
memory effects; iii) the model of advection-diffusion in a deforming porous medium (with no influence
of solid diffusion). Initially expressed by means of orders of magnitude of the diffusivity ratio,
the domains of validity of each of these three models can be expressed in terms of relative orders of
magnitude of two characteristic times. The three models contain a solute-solid interaction term, due
to the advection regime, and are coupled to the poroelasticity model via the advection term.

References:


Acceptance of Terms and Conditions:
Homotopy Continuation Method based on Dissipation Operator for Coupled Multiphase Flow and Transport in Porous Media

Author(s): Jiamin Jiang
Co-author(s): Hamdi Tchelepi

1 Stanford University

Corresponding Author(s): jiamin66@stanford.edu

In reservoir simulation, solving highly nonlinear algebraic equations arising from a fully-implicit discretization is challenging. There is generally no acceptable initial iterate available for multiphase flow and transport problems. Hence, a globalization strategy is usually needed when applying Newton’s method to the nonlinear system.

Homotopy continuation, which has been widely adopted in numerical algebraic geometry and bifurcation analysis, provides a promising way for globalizing Newton’s method. For a given nonlinear system to be solved, a homotopy between the given system and a new system (which is easier to solve) is constructed. Then the new system is gradually deformed into the original one along the homotopy through a path-tracking algorithm, thereby obtaining the solution to the original system.

In this paper, we develop a homotopy continuation method based on dissipation operator for solving multiphase flow and transport in porous media with combined viscous, gravitational and capillary forces. The homotopy is constructed by adding numerical dissipation to the discrete flow equations, with a continuation parameter controlling the magnitude of the dissipation. Numerical evidences and detailed analysis are provided through single-cell and 1D examples to illuminate why the dissipation operator can significantly improve the nonlinear convergence of hyperbolic PDE problem. In addition, an adaptive strategy to determine optimum dissipation coefficient is proposed. The adaptive dissipation is computed in a face-wise manner and is applicable to coupled flow and transport.

We demonstrate the efficacy of the new nonlinear solver using several numerical examples, including 1D scalar transport and 2D heterogeneous problems with fully-coupled flow and transport. The dissipation operator is found to be highly effective in resolving the specific convergence difficulty associated with the low wave speed around saturation front. Overall, the new solver exhibits superior convergence properties compared to the standard Newton’s method. Moreover, the new solver works robustly for a wide range of flow conditions without parameter tuning in the dissipation operator.

References:

Acceptance of Terms and Conditions:

Click here to agree

How does pore size distributions affect the accumulation and release rates of a PAH in porous media of sediments and soils?

Author(s): Gonzalo Jayme-Torres

Click here to agree
Co-author(s): Axel Falcón-Rojas 1; Adriana Villa-Navia 1; Jessica Arleth Hernández-Martínez 3; Anne M. Hansen 2

1 UNAM
2 IMTA
3 UPEMOR

Corresponding Author(s): gonzalojayme@hotmail.com

In areas contaminated by the petroleum industry, persistent compounds such as polyaromatic hydrocarbons (PAH) are often accumulated in the porous matrixes of sediments and soils (S&S), implicating risks to ecosystems and human health since these contaminants are released over time to interstitial and surrounding water. Pore size distributions (PSD) and PAH binding strengths to sorption sites on S&S are characteristics that affect such accumulation and release. Sorption, desorption and diffusion are among the critical processes that control the availability of PAH, and it is therefore crucial to evaluate these processes in order to understand and predict transport and fate of these contaminants in S&S, and for selecting effective remediation procedures.

Four S&S samples were obtained from previously contaminated sites, air-dried, and sieved (mesh 200), and organic matter (OM) was reduced in subsamples by hydrogen peroxide treatment, resulting in eight different porous media. Surface areas and PSD were determined (Autosorb IQ2MP, Florida), and OM was estimated by calcination (ASTM, 1993). Benzo(a)pyrene (BaP) was selected as study PAH and adsorption experiments were carried out in the dark with S&S suspended in NaCl (I=0.047 M) solutions, by adding five different concentrations of BaP with 7-14C-BaP as radioactive tracer, between 2.59 and 12.6x10-4 mmolBaP/gS&S, according to TG 106 Guideline (OECD, 2000). Reactors were fed with CO2-free air to keep suspensions oxygenated and allow carrying 14CO2 and stable CO2, produced by mineralization of BaP and OM, respectively, to alkaline traps, where CO2 production was measured by changes in electrical conductivity. Supernatant aliquots in the reactors and alkaline traps were obtained and 14C was measured in a liquid scintillation counter (Beckman Counter LS6500). At the end of the BaP adsorption experiments (14 d), 6.5 cm2 polyoxymethylene (POM) was added as a passive sampler, desorbing BaP from S&S. POM-accumulated BaP was extracted with acetone and sonication (EPA, 2007). 14C was quantified in the extracts as described above.

In the case of samples with complete organic matter, sorption at 14 days varies between 91.5 and 95.8%, while in the samples with reduced organic matter a variation between 78.7 and 89.9% was observed. Desorption velocities were much slower than adsorption rates, finding values between 2.0 and 6.0 % in 14 days and between 2.2 and 11.1% in 43 days. Using these values it is estimated that the time required to desorb BaP varies between 644 and 8,290 days. This difference between rates of adsorption and desorption should be considered when planning remediation actions for contaminated sites.

Two different time dependencies were observed in adsorption and desorption kinetics: a fast step considered to be due to diffusion of the BaP to the external surface, macro and mesopores, and a slow step, considered as diffusion of BaP into the micropores capillaries. Sorption equilibrium constant (KL), sorption sites and kinetic constants were experimentally obtained and a two-step conceptual model that describes the effect of the dynamics in porous media on the reactive transport of BaP in S&S with different PSD was developed.

References:
Click here to agree

Poster 1 / 1010

How does pore size distributions affect the accumulation and release rates of a PAH in porous media of sediments and soils?
Author(s): Gonzalo Jayme-Torres ¹
Co-author(s): Axel Falcón-Rojas ²; Adriana Villa-Navia ¹; Jessica Arleth Hernández-Martínez ³; Anne M. Hansen ²

¹ UNAM
² IMTA
³ UPemor

Corresponding Author(s): gonzalojayme@hotmail.com

In areas contaminated by the petroleum industry, persistent compounds such as polyaromatic hydrocarbons (PAH) are often accumulated in the porous matrix of sediments and soils (S&S), implicating risks to ecosystems and human health since these contaminants are released over time to interstitial and surrounding water. Pore size distributions (PSD) and PAH binding strengths to sorption sites on S&S are characteristics that affect such accumulation and release. Sorption, desorption and diffusion are among the critical processes that control the availability of PAH, and it is therefore crucial to evaluate these processes in order to understand and predict transport and fate of these contaminants in S&S, and for selecting effective remediation procedures.

Four S&S samples were obtained from previously contaminated sites, air-dried, and sieved (mesh 200), and organic matter (OM) was reduced in subsamples by hydrogen peroxide treatment, resulting in eight different porous media. Surface areas and PSD were determined (Autosorb IQ2MP, Florida), and OM were estimated by calcination (ASTM, 1993). Benzo(a)pyrene (BaP) was selected as study PAH and adsorption experiments were carried out in the dark with S&S suspended in NaCl (I=0.047 M) solutions, by adding five different concentrations of BaP with 7-14C-BaP as radioactive tracer, between 2.59 and 12.6x10^-4 mmolBaP/gS&S, according to TG 106 Guideline (OECD, 2000). Reactors were fed with CO2-free air to keep suspensions oxygenated and allow carrying 14CO2 and stable CO2, produced by mineralization of BaP and OM, respectively, to alkaline traps, where CO2 production was measured by changes in electrical conductivity. Supernatant aliquots in the reactors and alkaline traps were obtained and 14C was measured in a liquid scintillation counter (Beckman Counter LS6500). At the end of the BaP adsorption experiments (14 d), 6.5 cm2 polyoxymethylene (POM) was added as a passive sampler, desorbing BaP from S&S. POM-accumulated BaP was extracted with acetone and sonication (EPA, 2007). 14C was quantified in the extracts as described above.

In the case of samples with complete organic matter, sorption at 14 days varies between 91.5 and 95.8%, while in the samples with reduced organic matter a variation between 78.7 and 89.9% was observed. Desorption velocities were much slower than adsorption rates, finding values between 2.0 and 6.0 % in 14 days and between 2.2 and 11.1% in 43 days. Using these values it is estimated that the time required to desorb BaP varies between 644 and 8,290 days. This difference between rates of adsorption and desorption should be considered when planning remediation actions for contaminated sites.

Two different time dependencies were observed in adsorption and desorption kinetics: a fast step considered to be due to diffusion of the BaP to the external surface, macro and mesopores, and a slow step, considered as diffusion of BaP into the micropores capillaries. Sorption equilibrium constant (KL), sorption sites and kinetic constants were experimentally obtained and a two-step conceptual model that describes the effect of the dynamics in porous media on the reactive transport of BaP in S&S with different PSD was developed.

References:
Click here to agree
How to Predict CO2 Foam Propagation Distance by Using Bubble Population Balance Model

Mohammad Izadi$^1$; SEUNG I. KAM$^1$

$^1$ Louisiana State University

Corresponding Author(s): mizadi3@lsu.edu

Although foams are known for effectively reducing gas mobility and enhancing oil recovery in many field applications, it is still not clear how far the injected fine-textured foams will propagate into the reservoirs. Lacking such a knowledge makes the design of foam field treatments difficult and often unreliable. The purpose of this study is to investigate CO2 foam propagation distance as a function of injection foam quality and injection total rate by using bubble population balance model. This study is believed to cover the steps needed from the pore-scale to field-scale events.

In order to meet the purpose, this study performs the following tasks: (i) fitting bubble population balance model to lab coreflood experiments and determining model parameters; (ii) establishing the mathematical framework to determine foam propagation distance during EOR processes; and (iii) characterizing foam propagation distance at different injection strategies. The laboratory data consists of three foam states (weak-foam, strong-foam, and intermediate states) as well as two different flow regimes (high-quality and low-quality regimes) of the strong-foam state.

The mobilization pressure gradient is one of the key model parameters to distinguish gaseous CO2 foams from supercritical CO2 foams. It is because, the mobilization pressure gradient being proportional to the interfacial tension, supercritical (or dense) CO2 foams exhibit much lower mobilization pressure gradient compared to gaseous CO2 foams, often with a couple of orders of magnitude difference.

The results show that the presence of three different foam states as well as two different strong-foam flow regimes (high-quality and low-quality regimes) plays a key role in model fit and field-scale propagation prediction. More specifically, this study finds that supercritical CO2 foams can propagate a few hundreds of feet easily, which is a few orders of magnitude higher than gaseous CO2 foams. For dry foams (or, strong foams in the high-quality regime), higher injection gas fractions result in shorter foam propagation distance, while for wet foams (or, strong foams in the low-quality regime) the propagation distance is not really sensitive to injection gas fractions. In addition, the higher injection rates (or pressures), the farther foams propagate – such an effect is shown to be much more pronounced for dry foams.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 3 / 661

How to sink: impact of fluids in soil liquefaction during earthquakes, computation of critical acceleration.

Cécile Clément$^1$; Renaud Toussaint$^2$; Einat Aharonov$^3$; Shahar Ben Zeev$^4$; Liran Goren$^1$; Stanislav Parez$^6$; Lacieł Alonso-Llanes$^3$; Ernesto Altshuler$^3$; Alfo Batista$^9$; Gustavo Sanchez$^9$; Menka Stojanova$^{10}$; Mohammed Bousmaha$^{11}$

$^1$ ICGS, Univ Strasbourg
$^2$ CNRS, ICGS UMR 7316, University of Strasbourg
$^3$ Hebrew Univ Jerusalem
$^4$ Hebrew Univ of Jerusalem, ICGS, Univ of Strasbourg
$^5$ Univ Ben Gurion Neguev
$^6$ Univ Prague
Corresponding Author(s): renaud.toussaint@unistra.fr

Soil liquefaction is a significant natural hazard associated with earthquakes. Some of its devastating effects include tilting and sinking of buildings and bridges, and destruction of pipelines. Conventional geotechnical engineering assumes liquefaction occurs via elevated pore pressure. This assumption guides construction for seismically hazardous locations, yet evidence suggests that liquefaction strikes also under currently unpredicted conditions. We show, using theory, simulations and experiments, another mechanism for liquefaction in saturated soils, without high pore fluid pressure and without special soils, whereby liquefaction is controlled by buoyancy forces. This new mechanism enlarges the window of conditions under which liquefaction is predicted to occur, and may explain previously not understood cases such as liquefaction in well-compacted soils, under drained conditions, repeated liquefaction cases, far-field liquefaction and the basics of sinking in quicksand. We next introduce viscous forces between grains and fluids, and examine how they modify the dynamics once liquefaction has been triggered.

These results may greatly impact hazard assessment and mitigation in seismically active areas.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 1100

Hybrid Mixture Theory Based Modeling of Ice-Recrystallization in Frozen Biopolymers Subjected to Freeze-Thaw Cycles

Ying Zhao¹ ; Pawan Singh Takhar¹

¹ University of Illinois

Corresponding Author(s): ptakhar@illinois.edu

The frozen food products are subjected to freeze-thaw cycles during storage and shipping. These cycles result in ice recrystallization, surface dehydration, and solute and moisture diffusion, which damage the foods quality. The re-crystallization phenomena involves multiscale characteristics spanning from the scale of polymers to macroscale. The transport of moisture and vapors is complicated by diffusion of solutes governed by Gibbs free energy gradients in the matrix. This presentation will discuss the Hybrid Mixture Theory based equations used to model water, vapor, heat and solutes transport. The unsaturated transport equations will be coupled to phase change equations for predicting the crystal growth at nucleation sites. The effect of freeze-thaw cycles on crystal growth, which causes damage to the surrounding matrix will be discussed. For model validation, the predicted crystal growth/decay will be compared to the experimental porosity measured using X-ray micro-computed tomography (CT). The analysis of micro CT images to calculate porosity, tortuosity and pore size distribution will be presented.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-C / 36
Hybrid Modelling of Fractured Reservoirs Using the Effective Medium Theory

Daniel Wong\(^1\) ; Florian Doster\(^1\) ; Sebastian Geiger\(^1\) ; Arjan Kamp\(^2\)

\(^1\) Heriot-Watt University
\(^2\) Total S.A.

Corresponding Author(s): s.geiger@hw.ac.uk

Naturally Fractured Reservoirs (NFR) are usually multiscale in nature and exhibit power law length distributions which do not possess any characteristic length scale, rendering the use of continuum methods such as the dual porosity model invalid due to the non-existence of Representative Elementary Volumes (REV) (Berkowitz, 2002). This necessitates the adoption of hybrid models that represent a subset of the fractures as continua and the remainder as discrete fractures. However, the appropriate partitioning of fractures into these two subsets is an unresolved issue.

In this regard, we propose a workflow which utilizes the Effective Medium Theory (EMT) by Sævik et al. (2013) as both an upsampling tool and a partitioning guide for single porosity hybrid modelling. EMT is used to find the largest non-percolating subset of small fractures which will be upscaled into a single porosity background. The remaining fractures will be represented explicitly through the Embedded Discrete Fracture Matrix (EDFM) method (Lee et al., 2001). This workflow allows reservoir engineers to systematically design appropriate partitioning strategies for hybrid modelling within a matter of seconds without the need for trial and error.

The workflow is benchmarked via a two-part study. Part one validates the accuracy of EMT for fracture subset upsampling by comparing results generated from EMT against numerical upsampling via EDFM. The benchmark shows that EMT efficiently produces accurate fracture subset permeabilities and percolation thresholds. Part two compares simulation results generated from different partitioning choices. Single porosity hybrid models are generated using a sequence of upsampling sizes and then subjected to pressure drawdown. Pressure distributions and flowrates are then compared. The results show that hybrid models are accurate, in comparison to the fully resolved model, provided that the upsampling size is below the aforementioned percolation threshold. Altogether, these results show that the workflow is an effective approach to systematic hybrid modelling.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 503

Hybrid machine learning/adjoint sensitivity model for source zone sampling optimization

Tian Tang\(^1\) ; Masoud Arshadi\(^1\) ; Eric Miller\(^1\) ; Linda Abriola\(^1\)

\(^1\) Tufts University

Corresponding Author(s): tian.tang@tufts.edu

Modeling DNAPL source zone plume evolution using traditional flow and transport models is a computationally intensive process that requires specification of a large number of material properties and hydrologic/chemical parameters. Given its computational burden, Monte Carlo simulation using such models is particularly ill-suited for uncertainty assessment and/or subsurface sampling optimization in real field applications. In this work, we present an innovative approach that couples machine learning, adjoint sensitivity theory, and statistical analysis to optimize borehole sampling for quantification of the evolution of down gradient flux-averaged concentration.
Probabilistic models, based on discriminative random fields (DRF), are first employed to synthesize stochastic realizations of a subsurface source zone consistent with known, limited, site characterization data. Using a suite of full scale simulations as training data, a statistical model is developed to predict the spatial distribution and uncertainty associated with key features (i.e. permeability and sequestered contamination [aqueous, sorbed, and NAPL]) that control plume evolution and persistence. Given an initial spatial distribution of contaminant mass, conditioned on measured field data, the adjoint state sensitivity method is then employed to quantify the importance of local system properties on down gradient flux-averaged concentration. The optimal sampling design problem is then addressed using first-order second-moment uncertainty analysis. In the decision process, the costs of additional measurements are justified by a sufficient decrease in the uncertainty, selecting measurements associated with the highest expected worth.

The utility of this probabilistic statistical modeling approach is demonstrated using numerically generated, two-dimensional, heterogeneous DNAPL source zones. Results reveal that down gradient flux-averaged concentration sensitivities to initial contaminant mass compartments are strongly affected by local permeability values. In addition, initial aqueous and sorbed concentrations and their corresponding variances have a major impact on down gradient flux-averaged concentration at early times, while the influence of initial NAPL saturation persists for a longer period. This innovative sampling strategy, coupling sensitivity analysis and uncertainty quantification, shows promise for enhancement of our ability to guide characterization of source zones under realistic field conditions.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-C / 189

Hybrid-dimensional two-phase flow in fractured porous Media with interfacial pressure and saturation unknowns

Joubine Aghili¹ ; Konstantin Brenner² ; Julian Hennicker³ ; Roland Masson⁴

¹ University Côte d’Azur, LJAD-Inria-CNRS
² LJAD, Université de Nice Sophia Antipolis
³ University of Geneva
⁴ LJAD

Corresponding Author(s): roland.masson@unice.fr

We consider in this work, the extension to two-phase Darcy flows of the discontinuous pressure models in which the (d-1)-dimensional flow in the fractures is coupled with the d-dimensional flow in the matrix. The model accounts accurately for gravity effects inside the fractures, for discontinuous capillary pressure curves at the matrix fracture (mf) interfaces and for both drains and barriers. This can be achieved thanks to interfacial pressure and saturation unknowns accounting for the nonlinear two-phase Darcy flux conservation equations at mf interfaces. The first objective of this talk is to compare this model with more usual hybrid-dimensional approaches based on the elimination of the interfacial phase pressures using the linear single phase Darcy flux conservation equation at the mf interfaces for each phase or alternatively the pressure continuity assumption in the case of fractures acting as drains. Our second objective is to discuss discretization and solution strategies for this type of models.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 5-A / 550

Hydraulic Conductivity of Coarse Sand Affected by Trapped Air Bubbles

Tomas Princ1 ; Helena Maria Reis Fideles2 ; John Koestel3 ; Michal Snehota4

1 Czech Technical University in Prague
2 UFRJ, Universidade Federal do Rio de Janeiro, Brazil
3 Swedish University of Agricultural Sciences, Uppsala
4 Czech Technical University in Prague, Civil Engineering

Corresponding Author(s): tomas.princ@fsv.cvut.cz

The aim of this study was to experimentally determine a relationship between gas residual saturation (SGR) and corresponding hydraulic conductivity (K) of two coarse sands. The SGR indicates the ratio of volume of entrapped air bubbles to pore volume of the sample. Series of constant head infiltration-outflow experiments were used to determine the relationship between the K and the SGR. Air trapping was achieved by repeating drainage and imbibition of water into the initially fully saturated sample. The value of K was determined using a constant head infiltration experiment and evaluated by Darcy’s law from measured steady-state flux. After the first constant head infiltration run and then after each subsequent infiltration run, the sample was drained under tension (~30 cm, -50 cm) on a sand tank. The SGR was determined gravimetrically after each infiltration run. Each infiltration run thus provide one value of K(SGR).

First batch of experiments were done in a laboratory and K(SGR) relationship was obtained. Selected five samples were scanned by micro-computed x-ray tomography (CT) to obtain information on entrapped air cluster size, shape and distribution. For the second batch of samples, CT revealed that fractures that occurred in the lower part as a result of deformation of insufficiently rigid supporting textile mesh at the bottom of the sample. Therefore, the experimental setup with more rigid support, formed by thin carbon rods, was designed. The fractures were not observed when improved set-up was used for experiments and the K(SGR) relationship was similar to first and second batches of samples.

The spatial distribution of air bubbles within the sample, the histogram of air bubble sizes and residual air content were obtained from binarized CT images. It is clearly visible that the bubbles formed in globular cavities in the loosely packed sand. The cavities emerged as a result of sand particles displacement by growing bubbles.

Results confirmed the trend of decreasing K with increasing SGR for both sands under study. The highest entrapped air content and the largest bubbles were detected in the upper half of the sample. The results confirmed that the trend of the K(SGR) relationship was a consequence of changes in entrapped air bubbles distribution.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-C / 53

Hydro-mechanical coupling strategies for fluid-filled fractures using a hybrid dimensional formulation

Patrick Schmidt1 ; Holger Steeb1

1 University of Stuttgart

Corresponding Author(s): patrick.schmidt@mechbau.uni-stuttgart.de
Numerical investigations of subsurface flow in fractured porous media provide information about properties connected to underground matter and heat transport just as characteristics of fluid underground storage capacity. Many diffusion-based models in the literature precisely describe subsurface flow. Nevertheless, pronounced hydro-mechanically-coupled phenomena like inverse water level fluctuations (Noordbergum effect) cannot be reproduced by diffusion-based models alone. Direct Numerical Simulations of surface-coupled fluid-solid (fracture) interaction or coarse-grained continuum descriptions like Biot's theory are theoretically capable to reproduce such phenomena. However, in case of investigations of fractures with high aspect ratios (length vs. aperture, i.e. \(1/\delta > 1000\)) methods using explicit discretization of the fluid domain tend to fail due to technical discretization issues. By assuming a parabolic velocity profile, the hybrid dimensional approach avoids an explicit discretization of the fracture domain. Thus, the fluid domain's dimension is reduced by one and solved for the pressure as the only primary variable. The mass balance within the fracture is modified to take volume changes into account and realizes the interaction between both domains, namely the hybrid-dimensional and surrounding solid domain. The characteristics of the coupled system vary with the ratio of the compressibility of the fluid within the fracture and the dimension of the elastic moduli of the surrounding matrix. Principally, when the ratio of fluid compressibility and bulk modulus tend to one the coupled system becomes stiff. The challenge are consistent numerical implementations that guarantee conservation of global mass and convergence for the full bandwidth of property ratios. A staggered-iterative scheme is presented for systems using moderate fluid compressibilities. Both systems are solved independently, hence it allows the use of non-conformal meshes and achieves an increase in efficiency. For stiff systems, a fully coupled model formulation that uses coupled boundary elements in an implicit fashion is introduced. The fully coupled problem allows the modeling of complex fracture geometries since only one mesh for both formulations is needed. In the course of this work, two consistent coupling schemes using the hybrid-dimensional formulation coupled to a surrounding elastic bulk material are proposed. The work closes with a discussion of the numerical solution scheme by means of relevant simulations to validate the methods compared to a poroelastic formulation and investigations of different fracture patterns.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 205

Hydrogel based porous matrices for immobilization of bioactive molecules

Karolina Labus1; Łukasz Radosiński1

1 Division of Bioprocess and Biomedical Engineering, Faculty of Chemistry, Wroclaw University of Science and Technology

Corresponding Author(s): karolina.labus@pwr.edu.pl

Hydrogels are the specific group of hydrophilic porous materials, being composed of variety of natural, synthetic polymers or their combinations. Their characteristic feature is the possibility to swell in aqueous solutions. Moreover, the relatively high porosity and water content, softness, strength and the ability of various substances to diffuse through the pores of their cross-linked structure make the hydrogels valuable functional matrices for effective immobilization of different bioactive molecules, such as drugs, growth factors, cells and enzymes.

Presently, the main interest of industrial biotechnology is a production of valuable compounds with high efficiency, however at low cost and in a short processing time. Therefore, the practical use of immobilized enzymes finds profound economic justification. The most important advantages of such biocatalyst preparations is the increase in its stability, reusability and/or possibility to perform the process in a continuous system and significantly easier separation of the reaction products. Besides binding to insoluble carriers and crosslinking, the inclusion of enzymes (e.g. in hydrogel structures) is one of the basic types of immobilization. This method is relatively cheap, fast and enables to obtain active preparations with enhanced stability, without significant changes in the native structure of entrapped enzymes.
The parameters characterizing porous hydrogels as the effective enzyme carriers include: (i) type of used material (reversible or permanent gel), (ii) its molecular structure (linear polymer, blocks or grafted copolymer, poly-blend), (iii) origin (natural, synthetic or hybrid) and (iv) physicochemical properties (e.g. water absorption capacity, mechanical strength, resistance to increased temperatures and the quantity and quality of the reactive functional groups that could interact with molecules of caught biocatalyst). Among them, crosslinking degree, porosity and consequently the specific surface area potentially available for immobilized molecules seems to be a key factor.

The main aim of this research was to study the effect of preparation conditions on the porosity of obtained hydrogel matrices. For this purpose, different concentrations of applied polymers (gelatin, polyvinyl alcohol) and crosslinking agent (microbiological transglutaminase) were tested. The pore distribution in the studied hydrogel structures was examined using scanning electron microscopy (SEM). Subsequently, hydrogel matrices were tested for use as enzyme carriers. In this case, invertase from Saccharomyces cerevisiae was applied as the model biomolecule. Within this study, immobilization efficiency and the possibility of multiple use of such enzyme preparation were determined.

This research was performed a part of the project (2015/19/D/ST8/01899) supported by National Science Centre (Poland).

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-B / 866

Hydrogen storage, adsorption induced deformation and the role of confinement dimensionality in CAU metal organic frameworks

Margarita Russina; Veronika Grzimek; Gerrit Guenther; Moritz-Caspar Schlegel; Helge Reinsch; Norbert Stock

1 Helmholtz Zentrum Berlin
2 BAM Federal Institute for Materials Research and Testing
3 Institute of Inorganic Chemistry, Christian-Albrechts-University
4 Institute of Inorganic Chemistry, Christian-Albrechts-University Kiel

Corresponding Author(s): margarita.russina@helmholtz-berlin.de

We have studied mechanism of hydrogen storage in CAU-1 and CAU-8 metal organic frameworks synthesized at Christian-Albrechts-University of Kiel, Germany [1,2]. The structures of these compounds are built from aluminum polyhedra with fully coordinated metal ions. Using various types of organic linker molecules tunable structures with channels of different geometries, but very similar chemical composition can be formed. Thus, CAU-1 consists of a three-dimensional confinement network with cavities of 10 Å and 5 Å of average cross section, while the structure of CAU-8 contains one-dimensional channels of about 8 Å diameter.

We observed striking differences in hydrogen sorption of these compounds. CAU-1 exhibits a considerable hydrogen uptake reaching about 6 wt. % percentage at 50 K at the pressure of 1 bar which stays stable after several sorption cycles. Hydrogen uptake of CAU-8, in contrast, is substantially lower of only about 2.7 wt.% at 50 K and quickly erodes after few sorption/ desorption cycles. In order to understand the mechanism of such differences on the microscopic level we have conducted an extensive study using in-situ neutron scattering diffraction and spectroscopy [3]. We observe that hydrogen sorption in both compounds is driven by interactions between guest hydrogen molecules and the organic linkers having, however, a very dissimilar impact. In CAU-1, the adsorption of hydrogen on the organic linkers in the initial stages leads to the contraction of the framework structure and as a result to changes in the electronic potential landscape inside the pores. This in turn causes the increase of hydrogen uptake by triggering the rearrangement of the adsorbed molecules and the formation of additional occupied positions. Guest-host interactions in one-dimensional channels in CAU-8 lead high possibly to the partial collapse of one-dimensional channels and to the consequent decrease of hydrogen uptake. One can argue that a three-dimensional porous framework
could better resist an adsorption induced mechanical stress [4] as one-dimensional channel structures. Furthermore, smart tuning of adsorption-induced structural deformation of porous materials could be used for further improvement of storage capacities in metal-organic frameworks alongside with other recently reported approaches such as sorption of two hydrogen molecules at a single metal site [5].

References:

Parallel 4-B / 989

Hydromechanical couplings in multiphase granular systems: recent advances and perspectives

Bruno Chareyre¹ ; Chao Yuan² ; Eduard Puig Montella³

¹ Univ. Grenoble Alpes, 3SR lab. - France
² Univ. Grenoble Alpes, 3SR lab.
³ Univ. Grenoble Alpes, France / Polytechnic University of Catalonia, Spain

Corresponding Author(s): bruno.chareyre@3sr-grenoble.fr

This presentation report recent advances in the framework of the discrete element method (DEM) for multiphase granular media. Computationally efficient methods based on the DEM have been developed for a while for partially saturated materials but they have been generally limited to the pendular regime. In contrast, one hardly avoid expensive direct resolutions of 2-phase fluid dynamics problem for mixed pendular-funicular situations or even saturated regimes. Following previous developments for single-phase flow, a pore-network approach of the coupling problems is described. The geometry and movements of phases and interfaces are described on the basis of a tetrahedrization of the pore space, introducing elementary objects such as bridge, meniscus, pore body and pore throat, together with local rules of evolution ¹. As firmly established local rules are still missing on some aspects (entry capillary pressure and pore-scale pressure-saturation relations, forces on the grains, or kinetics of transfers in mixed situations) a multi-scale numerical framework is introduced, enhancing the pore-network approach with the help of direct simulations [2]. Small subsets of a granular system are extracted, in which multiphase scenario are solved using the Lattice-Boltzman method (LBM). In turns, a global problem is assembled and solved at the network scale, as illustrated by a simulated primary drainage.

References:

Click here to agree
Parallel 1-D / 510

INVESTIGATING UNDERGROUND CO₂ STORAGE IN POROUS MEDIA USING GEOLOGICAL LABS ON CHIP

Author(s): Anais Cario

Co-author(s): Abdou Khadid Diouf, Carole Lecoutre, Olivier Nguyen, Dominique Bernard, Yves Garrassos, Samuel Marre

ICMCB-CNRS

Corresponding Author(s): anais.cario@icmcb.cnrs.fr

CO₂ geological storage in deep saline aquifers represents a mediation solution for reducing the anthropogenic CO₂ emissions. So far, little is known about both the CO₂ storage impact on the underground geochemistry and on the microbial diversity inhabiting deep aquifers. Consequently, this kind of storage required adequate scientific knowledge and tools at the pore scale to evaluate injection scenarios or to estimate reservoir capacity. In this context, porous media designed inside high pressure / high temperature microfluidic reactors (micromodel or geological labs on chip – GLoCs) turn out to be excellent tools to complement the classical core-scale experimental approaches to investigate the different mechanisms associated with CO₂ geological storage in deep saline aquifers [2].

This talk will first highlight the latest results obtained at ICMCB concerning the application of the GLoCs to study the invasion processes of CO₂ in water and brine saturated GLoCs. In particular, direct optical visualization and image treatments allow following the evolution of the CO₂/brine phase distribution within the pores, including displacement mechanisms and pore saturation levels [3]. We will then present some ongoing work aiming at integrating in situ spectroscopy techniques in HP microreactors to get information about the dissolution and mineralization trapping. We have developed an experimental set-up to recreate 3D reactive porous media within a microfluidic channel (fixed packed bed of calcium carbonate – CaCO₃ microparticles). Thanks to X-ray laminography carried out at the European Synchrotron facility (ESRF), we have observed on reconstructed 2D images, the dissolution phenomena occurring during the successive injection of constant volumes of non-equilibrium solution. This proof of concept has opened new possibilities for using this methodology to acquire kinetic data on 3D reactive front phenomena in porous media.

Eventually, we will introduce the use of GLoCs as a significant tool to mimic the in situ biogeological reservoirs conditions to study CO₂ bioconversion (in the frame of the ERC project “Big Mac”). Indeed, beyond CO₂ geological storage investigations, the GLoCs could provide new insights into bioremediation process to restore the CO₂ as a valuable energy resource (i.e. CH₄ via methanogenesis process). These tools could also find wider applications in geological-related studies such as Enhanced Oil Recovery, shale gas recovery or geothermal energy.

References:


Parallel 7-H / 525

Identification of individual fibers from 3d digital images

Author(s): Andreas Grießer, Rolf Westerteiger

Co-author(s): Christian Wagner, Hans Hagen, Andreas Wiegmann

Click here to agree
Corresponding Author(s): andreas.griesser@math2market.de

Fibrous structures are present in many materials, including non-woven filter media used for filtration, carbon-fiber reinforced plastics or glass-fiber reinforced plastics used in mechanical applications, or gas-diffusion layers used in fuel cells. Spatial distribution, orientation, length, curvature and center line of fibers in materials like these are essential characteristics needed to know in modern material design. Being able to analyze these properties from micro-CT scans is highly important to create precise models of existing materials.

Most algorithms currently used to extract the statistics of the fiber orientations [1, 2, 3] first split the image space into many small fiber segments and try to recombine the over-segmented fiber segments afterwards. These methods lack accuracy, because they often connect fiber center lines incorrectly. The center line determination is especially challenging in places where two or more fibers touch.

We propose a machine learning based algorithm to identify and extract the individual fibers in segmented 3D images to be able to fully characterize the fibers and the overall composition of a material. Machine learning based on deep neural networks requires massive amounts of training data, in our case known fiber center lines. One approach could be to create these manually. However, this is not feasible for 3D data sets. Instead, we use GeoDict’s [4] fiber modelling capabilities and scripting capabilities to generate training data sets, which consist of voxelized 3d fiber models and analytically known fiber center lines.

When applied to a micro-CT scan, the trained neural network first labels the contact voxels (or bond points in the case of bonded fibers) between two fibers. Second, the labeled contact voxels are removed from the segmented image. In the final step, the resulting connected components are analyzed, and a skeleton-based approach is used to obtain analytic descriptions of every fiber. The center lines can then be used to analyze the material, e.g. to find spatial distributions, fiber orientation, fiber length, fiber curvature, etc. It is also possible to create a beam element model of the original micro-CT scan.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-H / 316

Image analysis, microstructure generation and effective property estimation of cement-based materials used as radioactive waste confinement barriers

Author(s): Laurent Lemmens1
Co-author(s): Bart Rogiers2; Eric Laloy2; Diederik Jacques2; Mieke De Craen2; Li Yu2; Tri Phung Quoc2; Rudy Swennen2; Guillaume Desbois1; Janos L. Urai2; Marijke Huysmans2

1 SCK-CEN / KU LEUVEN
2 SCK-CEN
3 KU Leuven
Transport through cement-based materials depends strongly on their 3D microstructure. To evaluate transport and related processes at time and spatial scales beyond experimental data, and to gain in depth understanding of the critical role of the microstructure, numerical simulations are necessary. This, however, requires an accurate description of the 3D microstructures involved. However, for cement paste, 3D imaging techniques such as µCT do not have sufficient resolution to appropriately describe the microstructure. We therefore present a new 3D-multiphase stochastic reconstruction methodology based on simulated annealing. Our methodology uses a single or set of 2D SEM images to calculate different 2D structural descriptors which are then fitted by a multi-phase simulated annealing-based reconstruction algorithm. This approach is easily extendible for generating 3D microstructures, by assuming isotropy. We demonstrate our approach for ordinary Portland cement pastes with different water to cement ratios. We evaluate the reconstruction methodology by calculating diffusion coefficients with a pore-scale transport model using a lattice Boltzmann approach and the generated 3D reconstructions. Results seem to agree very well with the measured diffusion coefficients for the same cement pastes. This builds confidence in the adequacy of the proposed simulated annealing algorithm for generating 3D realizations of cement paste from a 2D image. The approach will further developed to simulate transport properties in evolving porous systems during degradation to evaluate the confinement properties of cement-based materials over larger time scales in e.g. the context of radioactive and hazardous waste management.

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 9-D / 214

Imaging the spatial distribution of geochemical heterogeneities in porous media: multidimensional flow-through experiments and inverse modeling

Massimo Rolle¹; Maria Battistel¹; Felix Onses¹; Jonghyun Lee²

¹ Technical University of Denmark
² University of Hawaii

Corresponding Author(s): masro@env.dtu.dk

The spatial distribution of physical and chemical heterogeneities is critical in many subsurface applications. For instance, the location of reactive minerals is a primary factor controlling the fate and transport of organic and inorganic pollutants in groundwater. A number of studies have focused on using hydrologic measurements and inverse modeling techniques to image physical heterogeneity and the spatial distribution of hydraulic conductivity. However, such approaches are not commonly applied to water quality parameters and reactive transport problems. A recent numerical study proposed a methodology to use distributed sensor data and inverse reactive transport modeling to characterize arsenic mobilization and distribution.

In this work we focus on imaging pyrite inclusions in saturated porous media and we combine experiments with forward and inverse reactive transport modeling. We studied the oxidative dissolution of pyrite in different experimental setups, including batch systems, 1-D column setups and 2-D flow-through chambers. Measurements of water quality parameters such as pH, dissolved oxygen, iron and sulfur were useful to formulate and constrain pyrite dissolution kinetics within a reactive transport modeling framework. In particular, spatially-distributed measurements of dissolved oxygen in the 1-D and 2-D setups were instrumental for imaging pyrite inclusions. Non-invasive optode sensors along the column setups and at different cross sections in the 2-D system allowed us to measure oxygen transport and consumption at high spatial resolution (2.5 mm spacing). The oxygen data were combined with inverse reactive transport modeling based on the Principal Component Geostatistical Approach (PCGA) [2]. The results show that the proposed methodology allows imaging both the spatial distribution and the concentration of single and multiple pyrite inclusions in the 1-D and 2-D experimental setups.

References:

Parallel 5-E / 367

Imbibition on the single-pore level: what happens in the absence of cooperative phenomena?

Martin Steinhart¹

¹ Universität Osnabrück
Commonly, studies on imbibition focus on porous matrices with bicontinuous morphology that contain spongy pore systems with neck-node morphologies. In this context, much attention has been paid to cooperative imbibition phenomena such as imbibition front broadening, viscous fingering, or avalanche-like relaxations of the imbibition fronts, which occur in systems of hydraulically coupled pores. Non-cooperative imbibition phenomena confined to the single-pore level have attracted less attention. However, even the invasion of a separate cylindrical pore by a wetting liquid is accompanied by wealth of complex physical phenomena. Even though effects related to local variations in the Laplace pressure across the menisci at the imbibition front are absent, the transition from an empty cylindrical pore to a filled cylindrical pore is characterized by complex kinetics and the possible occurrence of long-lived metastable or transient imbibition morphologies. Theoretical treatment of single-pore imbibition has remained demanding, and predictive understanding of single-pore infiltration is premature. However, model systems allow experimentally capturing insights into single-pore imbibition. The infiltration of polymeric melts into self-ordered nanoporous anodic aluminum oxide (AAO) is an example for a revealing model scenario. AAO contains arrays of straight, separated cylindrical nanopores with narrow pore size distribution. The pore diameters range from 20 nm to 400 nm, the pore depths may amount up to 100 microns. Infiltration takes place on time scales convenient for laboratory experiments. If polymers with high glass transition temperature are infiltrated, transient infiltration stages can easily be frozen by vitrification of the polymer. Limiting cases are infiltration via intermediate precursor films on the pore walls and classical capillary infiltration by propagation of a thread of the invading liquid. Neither the transition between precursor film wetting and capillary wetting, nor the transition from a precursor film scenario to complete pore filling is satisfactorily understood. In this talk, the current state of knowledge concerning infiltration of AAO with polymers will be summarized with a special focus on known transient infiltration states, such as precursor film thickening and precursor film instabilities.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-D / 610

Impact of 3D capillary heterogeneity and bedform architecture at the sub-meter scale on CO2 saturation

Luca Trevisan¹ ; Timothy Meckel² ; Prasanna Krishnamurthy²

¹ Karlsruhe Institute of Technology
² The University of Texas at Austin

Corresponding Author(s): luca.trevisan@kit.edu

During the post-injection and stabilization period of geological carbon sequestration, the primary forces governing CO2 migration and entrainment are capillarity and buoyancy, delineating a specific field of application for numerical flow models. In contrast with conventional modeling approaches that assume laminar viscous flow regime, a modified invasion percolation (MIP) simulator is used to mimic the physics of fluid flow for vanishing pressure gradients. The current investigation extends a previous study simulating 2D CO2 invasion through stochastic and natural geologic models. Research presented here expands methods for addressing role of heterogeneity on fluid migration by quantifying the influence of 3D variability in threshold capillary pressure and bedform architecture on CO2 saturation. The goal is to develop a predictive method for volumetric storage capacity for buoyant flow conditions. Realistic sedimentary models are generated for eight common clastic facies with accurately represented bedform morphology. Resulting 3D models consist of matrix and lamina cells that are populated independently with probability density functions representative of sandstone lithologies with different grain sizes and sorting. Results from thousands of MIP simulations reveal saturation in the eight models to be a non-linear function that is primarily influenced by the contrast in threshold capillary pressures between matrix and lamina (observable lithologic
heterogeneity), suggesting some predictive ability is achievable from common sedimentologic descriptors, although quantifying the independent effect of depositional architecture remains more difficult.

**References:**


Meckel TA, Trevisan L, Krishnamurthy PG. A method to generate small-scale, high-resolution sedimentary bedform architecture models representing realistic geologic facies. Scientific Reports. 2017 Aug 23;7(1):9238. **Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 4-E / 40**

**Impact of CO2 Injection on Condensates Recovery from Shale Organic Nanostructures**

SEUNGHWAN BAEK1 ; I. Yucel Akcutlu1

1 Petroleum engineering, Texas A&M University

**Corresponding Author(s):** sbaek@tamu.edu

Compositional variation in multi-component system caused by adsorption and confinement in organic nanopores leads to capillary condensation and trapping of concentric hydrocarbon liquids. The objective of this paper is to show the presence of capillary condensation in kerogen pores, and argue that pressure depletion/liquid expansion is no longer effective and EOR process is required for these pores. We quantify stripping effects of CO2 on the condensates recovery from the kerogen nanopores and discuss the fundamentals of cyclic-CO2 injection into source rocks. Investigation is carried out using a multi-component hydrocarbon mixture representing fluids produced from US shale gas plays. Nano-channels in equilibrium with bulk phase such as fractures represent kerogen nanostructures and are modeled with varying sizes. Using Monte Carlo simulation, in-situ molecular configuration inside the nano-channels is restored as the pressure of the bulk phase and proportion of CO2 in bulk phase changes in stages. This process enables to correlate the accessible information, such as the subsurface conditions, produced bulk fluid composition and injected CO2 amounts, to inaccessible information such as the in-situ thermodynamic state of the hydrocarbon fluids and CO2 in kerogen. Based on information obtained from this, the impact of CO2 injection on recovery is systematically analyzed. Since selective adsorption of CO2 to kerogen is weaker than those of the heavy molecules in the mixture while stronger than those of the light components, it is difficult for the injected CO2 to strip off many hydrocarbons in small pores. For large kerogen pores, however, the injected CO2 relatively easily extracts the hydrocarbons from the pores. This in turn drives a shift in phase equilibrium properties and prevents the capillary condensation. Consequential significant enhancement in recovery is observed. Moreover, the higher injection pressure leads to the higher recovery in the small pores providing that the introduced CO2 takes up more than 50% of the bulk space. This is in contrast to the case of large pores that the injection following pressure depletion is preferred to enhance the recovery. An efficiency of the CO2 injection is generally improved as the pressure increases in small pores but it is still less effective than that in larger pores and the increasing pressure does not bring out substantial rises in the efficiency in the large pores. 6nm and 10nm pores show residual oil saturation, which is less than 0.2 and the values remain more or less constant over the investigated pressure range whereas the value in 2nm pore varies depending on injection pressure and it increases by a factor of 1.9 as the pressure depletes from 3,500psi to 500psi. The effects of introduced CO2 on transport properties of the hydrocarbon fluids in kerogen pores and other injecting agents (N2 and CH4) on the recovery are also investigated. The present work provides an essential understanding of the role of CO2 in multi-component fluids and lays down the first principles of CO2 injection into shale gas/condensate reservoirs.

**References:**
Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-C / 172

Impact of Fluid-Driven Subcritical Crack Growth on Hydraulic Fracture Initiation and Growth

Guanyi Lu¹ ; Qiao Lu¹ ; Romain Priou² ; Elizaveta Gordelty² ; Gallyam Aidagulov³ ; Andrew Buner³

¹ University of Pittsburgh
² Schlumberger-Doll Research
³ Schlumberger Dhahran Carbonate Research

Corresponding Author(s): buner@pitt.edu

Most approaches to stimulation of horizontal wells bore rely on initiation and growth of more than one hydraulic fracture. In the ideal case, each perforation cluster generates at least one hydraulic fracture, and the fluid and proppant are uniformly partitioned among these entry points. Simulation of this richly-coupled process of multiple fracture growth is an active area of research. But how do these multiple fractures initiate in the first place? A combined experimental and modeling study have recently led to new understanding of the mechanisms leading to the initiation (or not) of multiple hydraulic fractures. Our results demonstrate time-delayed initiation at well bore pressures insufficient to generate instantaneous hydraulic fracture growth, and we argue this mechanism is essential for initiation of additional hydraulic fractures within a stage once the first one or two fractures begin taking enough fluid that the well bore pressure plateaus or declines. Understanding the origins and mechanistically modeling this time delay is important because developing strategies to reduce the delay time will lead to successful stimulation from a greater proportion of perforation clusters. Our results show that the time delay can be predicted, with the models relying on characterization of so-called static fatigue properties and/or subcritical crack growth properties of rocks. We will also show experimental evidence that the time delay can be reduced by changing fluid properties. For example, low viscosity fluids generate a shorter time delay in general and use of dilute HCl reduces the time delay in carbonate rocks.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-F / 641

Impact of disorder on pressure saturation curves, and graph theory shedding light on the life and death of capillary bridges and films pathways.

Monem Ayaz¹ ; Renaud Toussaint² ; Knut Jørgen Måløy³ ; Marcel Moura³ ; Gerhard Schäfer³

¹ IPGS
² IPGS, Univ Strasbourg, PoreLab, Univ Oslo
³ PoreLab, Department of Physics, University of Oslo
⁴ LHYGES, Univ. Strasbourg

Corresponding Author(s): renaud.toussaint@unistra.fr

We study experimentally and numerically drainage situation in a disordered porous medium. We show how the fractal dimension associated to capillary fingering, the Bond number and fluctuations
amplitude in capillary thresholds allow to compute the residual saturation under various gravitational fields, and in various disordered distributions for the capillary thresholds. We also show how these parameters can allow to compute saturation-pressure curves for a given medium, and how the size of the chosen representative elementary volume has to be taken into account when using such curve. In the experiments, we study the residual saturation left behind as a fully saturated porous media is drained on a quasi two-dimensional porous model. The model is transparent, allowing the displacement process and structure to be monitored in space and time. Slow transport are aslo studied directly past a primary invasion front: Observations show the residual saturation to be interconnected by means of capillary bridges, allowing for seemingly entrapped fluid to be transported back to the bulk. This process shows dependence with the Bond number and a statistical decay with increasing distance from the invasion front. Furthermore we have analyzed the spatial connectivity of the networks spanned by capillary bridges, and examined the occurrence of rupturing of individual bridges. We characterize the dynamics of this slow transporting lowly connecting network of bridges and films using graph theory.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-F / 587

Impact of pore and pore-throat distributions on porosity-permeability evolution in heterogeneous mineral dissolution and precipitation scenarios

Jeffrey Steinwinder¹ ; Lauren Beckingham¹

¹ Auburn University

Corresponding Author(s): leb0071@auburn.edu

Mineral dissolution and precipitation reactions in porous media can alter formation properties, including porosity and permeability, in complex ways. While porosity increases with mineral dissolution and decreases with mineral precipitation, permeability alterations largely depend on the location of reactions in individual pores and the greater pore network. Pore network models enable simulation of permeability alterations from pore scale variations in dissolution and precipitation reactions. Uniform and non-uniform distributions of mineral reactions have been previously observed, controlled by pore size, PeDa, or mineral distribution, for example. In this work, the evolution of permeability with varying spatial reaction patterns is investigated for uniform, normal, and left and right skewed pore and pore throat size distributions using pore network modeling simulations. Simulated spatial reaction scenarios include uniform, random, channelized, and pore size dependent dissolution and precipitation reactions. Simulated permeability evolution is compared to permeability calculated using common macroscopic porosity-permeability relationships. These relationships are unable to reflect the evolution of permeability resulting from non-uniform structure modifications. For all pore and pore-throat distributions, the largest disagreement between the pore-scale simulations and the macroscopic relationships is for size-dependent reaction scenarios, where reactions initiate in small or large pores. Porosity-permeability evolution in these scenarios is step-like where reactions initiating in small pores have a region with large changes in permeability and little change in porosity and reactions initiating in large pores have a region with large changes in porosity and little change in permeability. These relationships are fundamentally different than the macroscopic relationships examined here. Simulation observations from the four pore and pore-throat size distributions will be leveraged here to develop new porosity-permeability relationships for these scenarios.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 2-C / 943

Impact of stacked geologic sequence on oil spill volumes

Florencia Vasquez\textsuperscript{None} ; Ipsita Gupta\textsuperscript{None}

Corresponding Author(s): fvasqu1@lsu.edu

Deepwater horizon/Macondo event, which occurred on April 20, 2010, was one of the most catastrophic scenario in the United States deep waters. After that situation, regulations for drilling and completion projects became more rigorous and worst-case discharge calculations are mandatory as part of an Oil Spill Response Plan. Drilling projects in deep water offshore is a huge investment for a company, and they are exposed to some risks. While drilling, an uncontrolled wellbore flow event could happen with a high discharge of liquid hydrocarbons into the environment. It is known as the worst-case discharge (WCD) scenario. Knowing in advance the total of potential volumes discharged will allow interceding from the surface and drill a relief well. Some reservoir parameters might impact more than others during a blowout. The impact of multiple stacked reservoir/non-reservoir formation on oil spill volumes/rates is investigated. Preliminary results suggest that although oil spill occurs from the hydrocarbon reservoirs, the geologic sequence impacts the amount of oil spilled.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-A / 452

Impact of surface complexation and electrostatic interactions during pH fronts propagation in silica porous media: Experiments and model based interpretation

Author(s): Lucien Stolze\textsuperscript{None}

Co-author(s): Muhammad Muniruzzaman \textsuperscript{1} ; Massimo Rolle \textsuperscript{2}

\textsuperscript{1} Geological Survey of Finland, Neulaniemietie 5, 70211 Kuopio, Finland
\textsuperscript{2} Technical University of Denmark

Corresponding Author(s): lucst@env.dtu.dk

Propagation of proton fronts exerts a fundamental control on geochemical processes and contaminant transport in subsurface systems (Muniruzzaman & Rolle, 2015). Protons are of key importance in pore water solutions since they affect the sorption behavior of charged contaminants by setting the surface charge at the mineral-liquid interface. Therefore, it is of primary importance to enhance our understanding regarding proton transport and complexation on mineral surfaces in order to accurately describe and predict reactive transport processes in porous media. Although significant effort, based on experimental studies and model development, has been dedicated to investigate pH sorption and surface complexation behavior in batch systems, only a few studies addressed the impact of these processes under flow-through conditions (McNeece & Hesse, 2016).

In this work, we systematically investigate the transport and sorption behavior of proton under flow-through conditions by means of laboratory experiments and reactive transport modeling. We performed experiments both in batch (titration) and in flow-through setups packed with saturated silica media (i.e. quartz sand and glass beads) with different grain sizes as porous matrix. Batch experiments were focused on characterizing and obtaining insights on the pH sorption capacities of the porous matrix and on the electrostatic interactions at the mineral pore water interface. Successively, we performed flow-through experiments in laboratory columns by applying continuous
injections of acidic solutions. Breakthrough curves of pH and all other major ions were measured at the outlet of the columns. In order to identify the importance of ionic strengths on charged species at the liquid-solid interface and on the multicomponent ionic transport, we performed parallel sets of analogous experiments (both in batch and column setups) with different background electrolyte solutions.

To quantitatively interpret the experimental results, we used a reactive transport model explicitly taking into account the triple-layer charge distribution multisite surface complexion (CD-MUSIC) model (Hiemstra & Van Riemsdijk, 1996) together with the Donnan approximation (Appelo & Wersin, 2007), and the cross-coupling of dispersive fluxes due to the Coulombic interactions between aqueous charged species (Rolle, et al., 2013). The modeling approach was based on a coupling between the geochemical code P4REEQC with MATLAB using IPHreqc module (Muniruzzaman & Rolle, 2016). The relative affinity constants of the surface complexion reactions were obtained through inverse modeling of the batch-titration and flow-through experiments. Experimental and modeling results suggest that the sorption behavior of protons differs in the considered silica porous media and are differently affected by the ionic strength of the background solutions.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 3 / 770

Impact of wellbore treatment fluids on calcium carbonate attachment in MICP grouted sands

Author(s): Fabian Steinacher

Co-author(s): Rebecca J Lunn 1; Grainne El Mountassir 1; James M Minto 1

1 University of Strathclyde – Department of Civil and Environmental Engineering

Corresponding Author(s): fabian.steinacher@strath.ac.uk

The interest in developing microbial induced carbonate precipitation as a cement alternative in oil and gas wells stems from the fact that this biotechnology can penetrate pore networks that conventional cement grouts cannot due to their high viscosity. Currently MICP is under investigation as a potential wellbore barrier technology to mitigate hydrocarbon leakage through a) micro-channels in the cement matrix b) micro-anuli as a communication pathway between the casing and the wellbore cement sheath c) and compromised wellbore cement sheaths. A major concern of this grouting technology is how to guarantee long-term well integrity. In particular, wellbore treatment fluids and multiphase subsurface fluids may interfere with carbonate production and/or attachment, thus compromising the integrity of the wellbore repair. In this research, we investigate the impact and influence of hydrocarbons and of currently available state-of-the-art wellbore treatment fluids and determine how these affect the performance of our “biomineral-seal” in the subsurface.
Biologically mediated calcium carbonate precipitation on grain surfaces within a sandy porous media, is known to cause several effects. Carbonates that precipitate in pore throats can form bridges in between the individual sand grains which results in increased strength of the porous media and some reduction in permeability. Carbonate biominerals that precipitate on grain boundaries within the pore space provide additional grain roughness, which leads to an increase in nucleation sites for further precipitation of calcium carbonate crystal polymorphs. Continued biomineral treatment results in a decrease in rock porosity.

The impact of hydrocarbons and other well-bore treatment fluids on biomineralization processes at the microstructural scale, including bacterial attachment and subsequent carbonate precipitation are largely unknown. In this experimental study, we explore the effect of biomineralization on the microstructural and physical properties of a series of batch cemented sand samples at elevated temperatures and pressures in the presence of hydrocarbons. We also explore, for the first time, the effect of wellbore treatments fluids.

We use Micro X-ray computer tomography to compute pore-structural properties (porosity, permeability, specific surface area and volume fraction of calcite attached to the sand grains). To investigate the attachment of precipitated carbonate and bacterial cells (entombed in calcium carbonate) to grain boundaries or calcium carbonate (free-floating) precipitated within pores, Scanning Electron Microscopy with Energy Dispersive X-Ray Spectroscopy (SEM-EDS) are deployed. In parallel, calcium carbonate crystal polymorphology is evaluated by X-ray diffraction (XRD) and, in case of hybrid crystal polymorphology, by Transmission Electron Microscopy (TEM).

Ongoing experiments focus on 1) investigating the survival of S. pasteurii in particular wellbore environments with well-known drilling fluids, corrosion inhibitors and hydrocarbons 2); identifying fluids that might negatively impact on attachment of calcium carbonate 3); the influence of key fluids on crystal polymorphology.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-D / 674

Impacts of Controlled Surface Roughness on Fluid Trapping in Glass Micromodels: Implications for Subsurface Multiphase Flow

Ayaz Mehmani\(^1\); Shaina Kelly\(^2\); Carlos Torres-Verdin\(^1\); Matthew Balhoff\(^3\)

\(^1\) The University of Texas at Austin
\(^2\) ConocoPhillips
\(^3\) University of Texas at Austin

Corresponding Author(s): mehmani.ayaz@utexas.edu

Pore-scale surface roughness occurs in varying degrees and forms within geologic media due to authigenic cement coatings and clay minerals. Such roughness increases the surface area contacted by fluids and chemical additives during subsurface operations such as enhanced oil recovery, storage of hazardous waste, carbon storage and sequestration, and non-aqueous phase liquid (NAPL) remediation from groundwater aquifers.

We utilize glass microfluidic chips (micromodels) to investigate the impact of surface roughness on trapped phase saturations after immiscible two-phase drainage and imbibition experiments. A new method is developed for incorporating surface roughness into glass microfluidic chips which allows tuning of roughness spatial distribution and height variation. Micromodels with rough and smooth surfaces are fabricated and light microscopy and image processing techniques are utilized to capture and quantify fluid phase distributions throughout each experiment. Imbibition experiments
are conducted by placings water droplets on the inlet port of the micromodels, whereupon the liquid spontaneously enters the chip. Air is injected at a constant flow rate into micromodels filled with crude oil to replicate drainage.

It is found that surface roughness with an average height of approximately 10% of the matrix pore depth increases trapped air saturation by ten to twenty times following spontaneous imbibition. This behavior is due to an increase in the occurrence of snap-off at throats and contact line pinning within pores that is enhanced by surface roughness. Drainage experiments are performed to investigate the impact of surface roughness on viscous fingering. Each micromodel is initially fully saturated with crude oil (100 centipoise viscosity) while air is subsequently injected at a constant flow rate. We find that the presence of surface roughness broadens the viscous fingering dendrites but trapped wetting phase saturation remains close to trapped saturation measured in smooth micromodels. Finally, we investigate the impact of surface roughness for a single fracture in a micromodel. This combination replicates the presence of large fractures within reservoirs and can have a significant effect on the efficacy of subsurface fluid production operations. We find that the roughness of large fractures does not affect trapped saturation significantly (less than 5%).

The various immiscible two-phase flow experiments considered in our work are valuable for determining the residual hydrocarbon saturation after water flooding a reservoir, establishing the flowback subsequent to hydraulic fracturing of a tight formation, and estimating the optimum injection volume for removing NAPL from aquifers. In addition, the method of incorporating controlled surface roughness into micromodels can be implemented as a tool for investigating surfactant absorption in chemical oil recovery, dispersion of carbon dioxide during carbon sequestration, and interpretation of tracer breakthrough profiles. Finally, the experimental results and workflow presented in this study can assist in verifying the reliability of numerical simulations of multiphase subsurface operations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 360

Impacts of Methane on Carbon Dioxide Storage in Brine Formations

Mohamad Reza Soltanian1; Mohammad Amin Amooie2; David Cole3; Thomas Darrah3; David Graham3; Susan Pfiffner4; Tommy Phelps1; Joachim Moortgat2

1 University of Cincinnati
2 The Ohio State University
3 Oak Ridge National Laboratory
4 University of Tennessee

Corresponding Author(s): m.rezasoltanian@gmail.com

In the context of geological carbon sequestration (GCS), carbon dioxide (CO2) is often injected into deep formations saturated with a brine that may contain dissolved light hydrocarbons such as methane (CH4). In this multicomponent multiphase displacement process, CO2 competes with CH4 in terms of dissolution, and CH4 tends to exsolve from the aqueous into a gaseous phase. Because CH4 has a lower viscosity than injected CO2, CH4 is swept up into a ‘bank’ of CH4-rich gas ahead of the CO2 displacement front. On the one hand, this may provide a useful tracer signal of an approaching CO2 front. On the other hand, the emergence of gaseous CH4 is undesirable because it poses a leakage risk of a far more potent greenhouse gas than CO2 if the cap rock is compromised. Open fractures or faults and wells could result in CH4-contamination of overlying groundwater aquifers as well as surface emissions. We investigate this process through detailed numerical simulations for a large-scale GCS pilot project (near Cranfield, Mississippi) for which a rich set of field data is available. An accurate cubic-plus-association (CPA) equation-of-state (EOS) is used to describe the non-linear phase behavior of multiphase brine-CH4-CO2 mixtures, and breakthrough curves in two
observation wells are used to constrain transport processes. Both field data and simulations indeed show the development of an extensive plume of CH4-rich (up to 90 mol%) gas as a consequence of CO2 injection, with important implications for the risk assessment of future GCS projects.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 376

Implicit Hybrid Upwinding for Multiphase Flow and Transport with Buoyancy and Capillary Pressure

Author(s): Francois Hamon¹
Co-author(s): Bradley Mallison ²; Hamdi Tchelepi ³

¹ Lawrence Berkeley National Lab
² Chevron
³ Stanford University

Corresponding Author(s):

The PDEs governing multiphase flow and transport in heterogeneous porous media are highly nonlinear. Therefore, in the fully implicit finite-volume method, solving the algebraic systems is challenging and accounts for most of the simulation cost. We present a numerical scheme applicable to general-purpose simulation that reduces the computational cost by improving the nonlinear convergence.

In the discretized transport problem, the interfacial approximation of the functions of saturation has a strong impact on the strength of the nonlinearities. We generalize an approximation method tailored to the multiphase physics and based on Implicit Hybrid Upwinding (IHU) that results in fast nonlinear convergence. This is achieved with a differentiable and monotone numerical flux for two-phase transport obtained from separate evaluations of the viscous, buoyancy, and capillary fluxes. Then, using IHU, we construct an efficient physically based discretization scheme for the mixed elliptic-parabolic problem in which the flow is coupled to the transport of species. Finally, to accurately represent capillary heterogeneity, the proposed scheme accounts for spatially discontinuous capillary pressure functions at the interface between different rock types thanks to discrete transmission conditions.

We present a mathematical analysis that places this new fully implicit finite-volume scheme on a strong theoretical foundation. The mathematical study is supported by challenging heterogeneous two-phase numerical tests demonstrating that the IHU scheme results in significant reductions in the number of nonlinear iterations compared to the commonly used phase-per-phase upstream weighting scheme for viscous-, buoyancy-, and capillary-dominated flow.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-H / 412

Improving the Monte Carlo algorithm for pore-network simulations of immiscible two-phase flow in porous media
Santanu Sinha¹, Alex Hansen²

¹ Beijing Computational Science Research Center
² NTNU

Corresponding Author(s): santanu.sinha@ntnu.no

Pore-network modeling provides a platform to study the upscaling problems in two-phase flow in porous media by representing the pore structure with a network of links and linking the pore-scale physics to the larger network. However, the bottleneck in this approach is the necessity to solve the pore-pressure field at each time step which makes it more and more computationally expensive with the increase of the network size. Moreover, when interested only on the steady-state properties, the advancing of interfaces using the time integration provides too much information about the transients. In order to improve the computational limitations inherent to the network models, we proposed a Markov Chain Monte Carlo algorithm based on the Metropolis algorithm for the pore-network simulation of two-phase flow under macroscopic steady-state conditions. The algorithm generates steady-state configurations of fluids based on configuration probability, and improves the computational time significantly compared to the time stepping. The results obtained with Monte Carlo are found in agreement with the time stepping, however, it uses a rectangular sub-system to generate trial the configurations which breaks the long range correlation at high saturation. A rectangular sub-system also limits the usability of the algorithm for a irregular networks, for example in case of the three dimensional networks reconstructed from real core samples. We will address this problem here, by replacing the rectangular sub-system with an irregular sub-network of flow highways, which can preserve the long range correlations of the flow and can improve the quality of the algorithm.

References:


Parallel 10-B / 875

In silico characterization of chloride-based salt hydrates for thermochemical heat storage

David Smeulders¹; Camilo RindtNone; Amar PathakNone; Silvia NedeaNone; Herbert ZondagNone

¹ Eindhoven University

Corresponding Author(s): d.m.j.smeulders@tue.nl

Thermochemical materials can store solar energy in the form of chemical energy. The stored solar energy can be used for household applications (hot tap water and room heating). These materials thus form a so-called heat battery. We investigate how salt hydrates can be used for this purpose. These salt hydrates release water (dehydration) when they absorb solar energy in summer. They absorb water (hydration) to release solar energy in winter. The durability and the rate of heat release (power) from the storage system depend on the chemical and physical properties of salt-hydrates. Magnesium chloride and calcium chloride hydrates are often used salt hydrates. There are, however, undesired chemical reactions which could occur during dehydration. One of them is the production of hydrochloric acid.

Using multi-scale modeling, Amar studied the salt hydrates in full atomic detail. From atomic modeling, he found out that CaCl2 hydrates have higher resistance to undesirable hydrochloric acid production than MgCl2 hydrates. On the molecular scale, material properties like diffusion coefficients and thermal conductivities of these salt hydrates are derived from the motion of atoms. These properties affect the performance of salt hydrate-based storage systems. Furthermore, the effects of cracks and defects, which are usually observed in experiments, on the dehydration reaction are investigated. The research also identified that a chemical mixture of CaCl2 and MgCl2 hydrates has
higher resistance to unwanted hydrochloric acid production than the hydrates of the pure components. In this way, an important step is made towards high-performance salt hydrate-based heat batteries.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-A / 137

In-situ and ex-situ dissolution for carbon dioxide sequestration

Yuri Leonenko

1 University of Waterloo

Corresponding Author(s): leonenko@uwaterloo.ca

It is widely excepted that CCS (Carbon Capture and Storage) could play a major role in mitigating climate change associated with CO2 emissions. Variety of industrial scale of CCS projects provide strong empirical support for the view that CO2 storage can be implemented safely. Nevertheless, many uncertainties remain regarding the security of underground storage. The major technical concern is the risks of leakage from the storage formation. Therefore, a critical issue for geological sequestration is to ensure that the stored CO2 does not escape from the underground formations. In conventional approach, after injection CO2 will slowly (scale of thousand years, [2]) dissolve in aquifer brine. During this time there is free CO2 available to leak. To eliminate or reduce the risks of leakage we proposed new methods to dissolve CO2: in-situ dissolution [3] and ex-situ dissolution aiming CO2 to be dissolved before it is injected underground [4]. In ex-situ approach brine produced from target aquifer is mixed with previously captured and liquefied carbon dioxide. After that carbon dioxide-brine mixture enters a pipe where the process of dissolution of carbon dioxide in brine occurs. After the dissolution process is completed in the pipe, CO2 saturated brine is injected back to the aquifer. During the dissolution process along the pipeline variety of dissolution regimes occur depending on CO2 droplet size and in our previous studies [4, 5] models for different regimes were developed. In the study presented here an overview of both methods is presented. Development of methods and tools to mitigate the risks of leakage provide great benefits for widespread of CO2 storage technologies, facilitating regulatory and policy decisions.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-B / 915

In-situ control of soft adsorbents pore size for optimal separation properties
Nicolas Chanut1 ; Sandrine Bourrelly2 ; Bogdan Kuchta2 ; Philip Llewellyn3

1 Massachusetts Institute of Technology
2 Laboratoire MADIREL
3 Aix-Marseille University

Corresponding Author(s): nchanut@mit.edu

Gas separation processes involving adsorption may have advantages over other separation methods although one drawback still remains the need for increased selectivity. A simple way to improve the selectivity of a separation process is to increase the pore confinement in the adsorbent. For instance, this can be achieved by the inclusion of large cations in the case of zeolites or by controlling the activation conditions of carbons. With flexible Metal-Organic Frameworks (MOFs), one can modify the chemistry to control the pore size or shape. These methods allow a primary control of the pore structure from the synthesis step. However, the question arises as whether it is possible to control the pore size or shape of existing porous adsorbents during the adsorption process via utilization of an external stimulus.

In this fundamental study, we have applied an external mechanical pressure to compress a flexible Metal-Organic Framework, MIL-53. Indeed, some MOFs are considered as soft porous crystals which can change reversibly their structure when they are exposed to stimuli such as adsorbed molecules1, pressure2 or temperature. This structural flexibility, leading to a change in the pore size, strongly influences the selectivity of the adsorbent for some gas mixtures. For example, the MIL-53 solid in its narrow pore form exhibits a very good CO2/CH4 selectivity, which is lost when the structure switches to the large pore form with the increase of gas pressure3. By maintaining the narrow pore form via mechanical compression, it may be possible to control its selectivity over a wider range of pressure or even induce molecular sieving. Releasing the mechanical pressure will lead to the large pore form which could be easier to regenerate.

For this purpose, we have developed a novel methodology to tune the adsorption behavior of mechanically responsive materials by coupling the effects of ‘internal’ gas adsorption pressure and ‘external’ mechanical pressure. In order to pilot the structural flexibility of the adsorbent during the gas adsorption, we built an experimental device to apply a mechanical pressure (up to 25 tons) on the porous material via a uniaxial press system which equally allows gas adsorption up to 15 bars. Results showing proof of concept with the MIL-53 will be given along with some openings towards more applied subjects.

References:

Click here to agree

Poster 4 / 856

Induced Seismicity in Subsurface Technologies: New Operational Constraints in Need of New Computational Models

Ruben Juanes1

1 MIT

Corresponding Author(s): juanes@mit.edu

The coupling between subsurface flow and geomechanical deformation is critical in the assessment of the environmental impacts of groundwater use, underground liquid waste disposal, geologic storage of carbon dioxide, and exploitation of shale gas reserves. In particular, seismicity induced by fluid
injection and withdrawal has emerged as a central element of the scientific discussion around subsurface technologies that tap into water and energy resources. Here we present a new computational approach to model coupled multiphase flow and geomechanics of faulted reservoirs. We present the application of the coupled flow-geomechanics simulation technology to the post-mortem analysis of several earthquake sequences. These early applications suggest that computational modeling of coupled flow and geomechanics, in combination with geologic, seismotectonic, and geodetic constraints, provides a promising approach for assessing and managing risk due to induced seismicity.

References:

Parallel 7-B / 111

Influence of RVE generation method on effective heat conduction modeling in open-cell ceramic foams: Review and recent advances

Author(s): Zi Kang Low

Co-author(s): Salvatore Cunsolo ; Nawfal Blal ; Naim Naouar ; Laurie San Miguel ; Dominique Baillis

1 Université de Lyon, INSA Lyon, LaMCoS CNRS UMR5259 ; Saint-Gobain C.R.E.E.
2 Université de Lyon, INSA Lyon, LaMCoS CNRS UMR5259
3 Saint-Gobain C.R.E.E.

Corresponding Author(s): zi.low@insa-lyon.fr

Ceramic foams play a crucial role in thermal engineering, as their porosity confers interesting properties which, combined with their high-temperature stability, allows them to meet both heat exchange and heat insulation demands. To facilitate optimization of the pore-scale morphology, numerous techniques have been developed to generate periodic representative volume elements (RVEs) of the foam mesostructure. As a fascinating variety of morphologies has been observed in ceramic foams, the choice of RVE generation method remains an open problem. In the present work, a review of available methods is performed to identify those most capable of reproducing the morphologies of real foams. Through a case study of conductive heat transfer modeling in an open-cell ceramic foam, the influence of RVE generation method is then analyzed.

In the context of heat transfer modeling, developments in RVE generation techniques are driven mainly by studies on radiative or convective transfer, where the effect of morphology is pronounced. Two main approaches to generate RVEs are distinguishable from the literature:

- The first treats the foam as a subtraction of elementary objects, usually spheres, from a solid phase. Early works assume regular packing (such as in face-centered cubic lattices), while recent developments introduce dispersity and contact laws to simulate bubble physics.
• The second approach partitions the volume into cells with minimum surface energy, then grows the solid phase from the cell faces (walls) and edges (struts). As with the first approach, regular partitions (such as the Kelvin cell) are increasingly being superseded by Voronoi-based structures that reflect the disorder in real foams.

In both approaches, physics-based techniques (bubble simulation or Voronoi-based tessellation) currently give the most realistic foam representations, often with predetermined cell size distributions as input. For open-cell structures, the key differences in the resulting geometries lie in the void phase connectivity and the range of pore and strut shapes possible. The Voronoi-based approach seems well suited to distinctively polyhedral pores. However, when the pores appear spherical (as is the case for many ceramic foams), both approaches have been successfully used to reproduce key morphological parameters of real foams. It is thus interesting to quantify the influence of the choice of RVE generation approach on the modeled effective thermal conductivity.

A case study is performed on an open-cell alumina foam with 80% porosity, with morphological parameters extracted from micro-tomographic images. Two periodic RVEs are then generated with state-of-the-art approaches, starting with random packing of non-overlapping, polydisperse spheres in a cubic volume. The first inflates the spheres before subtracting them from a solid matrix. The second uses the spheres as seeding points for a Voronoi-Laguerre diagram, to which polygonal struts of non-constant section are added. Both RVEs are geometrically validated with the morphological parameters of the real foam. Finite element modeling is used to obtain the effective thermal conductivity of the real foam mesostructure and the two RVEs. The RVEs may then be used to perform parametric studies on the foam morphology. The results highlight the influence of RVE generation technique, and provide modeling guidelines for future work.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-E / 718

Influence of layer charge location and inter-layer cations on swelling properties of mixed layer Illite-Montmorillonite

Mahsa Rahromostaqim\textsuperscript{1}; Muhammad Sahimi\textsuperscript{1}

\textsuperscript{1} University of Southern California

Corresponding Author(s): moe@usc.edu

Swelling of clay minerals play an important role in many fields including gas and oil industry and CO\textsubscript{2} sequestration. More than 60 percent of sedimentary samples in the US are of different types of mixed layer clays. We used molecular dynamics simulations to investigate the effects of layer charge location, interlayer cations (K\textsuperscript{+} and Na\textsuperscript{+}) and their concentration ratio on swelling of mixed layer Illite-Montmorillonite. Illite-Montmorillonite mixed layer consists of Illite-Montmorillonite and Montmorillonite-Montmorillonite interlayers. For all of the cases of this study, d-spacing was measured as a function of water content.
For Na-montmorillonite model with layer charge concentrated in the octahedral sheet, weak ion–surface interaction results in fully hydrated ions and therefore more swelling. This is in good agreement with the previous experimental and computational findings. However, in the asymmetric interlayer of mixed layer Na-illite-Montmorillonite, the Illite side with stronger surface-ion interactions results in a considerable cation concentration near the Illite surface. This limits hydration of cations and therefore controls swelling in mixed layer clays compared to the pure Montmorillonite interlayer. In addition, further inhibition of swelling from that of Na-mixed layer can be reached with increasing K\(^+\) to Na\(^+\) ratio in the interlayer. However, it was shown that increasing K\(^+\) fraction above 0.7 is not strongly felt by the mixed layer clays. Moreover, Clay hydration enthalpies, interlayer atomic density profiles and radial distribution functions are consistent with the swelling results in all cases.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Poster 3 / 603**

**Influence of micro-fabric heterogeneity on fracture alterations during shear**

Dustin Crandall\(^1\) ; Magdalena Gill\(^2\) ; Johnathan Moore\(^3\) ; Sarah Brown\(^4\) ; Laura Dalton\(^5\)

\(^1\) U.S. Department of Energy National Energy Technology Laboratory

\(^2\) AECOM and the National Energy Technology Laboratory

\(^3\) AECOM, National Energy Technology Laboratory

\(^4\) AECOM, contractor for NETL

**Corresponding Author(s):** dustin.crandall@netl.doe.gov

Because of the low permeability of shale, fractures typically act as the primary flow conduits in these formations. It is therefore imperative to understand the fundamental processes that influence fracture properties in shale to accurately predict unconventional resource production as well as ensure sequestered CO\(_2\) does not migrate out of a storage reservoir. In this study, a novel shearing apparatus was used in conjunction with a Hassler-style core holder to incrementally shear various shale cores while maintaining various confining pressures to simulate a fracture subjected to shearing forces. Intermittent computed tomography scans performed after each shearing event were used to obtain information on evolving fracture morphology. Transmissivity of the fracture was measured after each shearing event to better understand the hydrodynamic response to the evolving fracture morphology.

Two distinct shales were sheared using this process: a relatively homogeneous section of black Marcellus shale and heterogeneous subcores of Eau Claire shale. The heterogeneous Eau Claire shale exhibited more complex fracturing behavior with multiple secondary fractures. Fracture intensity throughout the samples was measured as a function of sheared differences and the relationship between micro-fabric complexity and fracture evolution is presented for these samples.

**References:**


**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 10-E / 818**
Influence of particle shape on reaction and transport patterns in fixed beds for methanol partial oxidation to formaldehyde

Behnam Partopour\(^1\) ; Anthony Dixon\(^1\)

\(^1\) Worcester Polytechnic Institute

Corresponding Author(s): bpartopour@wpi.edu

Formaldehyde is a very important chemical with a wide range of applications. Methanol partial oxidation on Fe-MoO\(_3\) catalyst is the most favorable method for formaldehyde production. The catalyst for this process is highly selective toward formaldehyde production (selectivity > 90\%). Methanol conversion in the process is also high (conversion > 98\%). The scholarly work on methanol partial oxidation has been mostly focused on the catalyst optimization, and very few studies have tried to evaluate the fixed bed performance and detailed interactions of fluid flow, reaction and transport in the system.

In this work we focused on the effects of the fixed bed configuration on the system performance, particularly, selectivity toward formaldehyde. To investigate the potential impact, a detailed computational method is developed to integrate the flow with the transport and reaction in both the fluid and solid phases. The catalytic particles with complex shapes are explicitly modeled using resolved-particle CFD simulations. Four different particle shapes are studied: sphere, cylinder, ring and tri-lobe. It is shown that the local selectivity is highly correlated with radial temperature gradient and particle shapes. Furthermore, the radial heat transfer is also affected by the particles shapes. The results suggest that particles with more area to volume ratio not only provide more surface for fresh feed to react but also due to shorter diffusion path prevent the formaldehyde from further oxidation. However, such particle shapes could negatively affect the radial heat transfer, and cause a higher radial temperature gradient. The results provide new insights for a better design and optimization of fixed bed processes.

Finally, the three-dimensional resolved-particle CFD results are compared with a standard 1-dimensional model. The limitations of the latter model are discussed and a resolution for their improvement is suggested.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 200

Influence of rock micro-pore structure parameters on Remaining oil Distribution

Author(s): Shuyao Sheng\(^1\)

Co-author(s): Yonggang Duan\(^1\) ; Tiantian Zhang\(^2\)

\(^1\) Southwest Petroleum University
\(^2\) PetroChina Turpan-Hami Oilfield Branch Engineering Technology Research Institute

Corresponding Author(s): 296634273@qq.com

Most of the water-flooding fields in the eastern part of our country have now entered the stage of high-water-cut mining, their actual recovery rates are generally low. Because of this, the research on the remaining oil distribution in the reservoir is urgent. In order to reflect the influence of the pore structure parameters of the core on remaining oil from the microscopic scale, this article starts with sandstone core. The displacement experiment of the selected rock samples and the micro-grayscale images of the cores were obtained after CT scanning. Then images are processed by non-local uniform filtering and watershed segmentation algorithm. Finally, some of the pore structure units were extracted from the remaining oil distribution obtained and a pore network model was constructed. Experimental results show: Rock pore radius is proportional to the degree of enrichment of remaining oil and inversely proportional to the water-flooding effect. The coordination number and shape
factor of rock are inversely proportional to the degree of enrichment of remaining oil and proportional to the water-flooding effect. What’s more, the pore-throat ratio value is more intermediate, the lower the enrichment of remaining oil, the better the water-flooding effect. This study is of guiding significance for the design of the remaining oil in the water-flooding oilfield.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-H / 740

Information-theoretic approach to conductivity upscaling

Daniel Tartakovsky¹; Francesca Boso¹

¹ Stanford University

Corresponding Author(s): fboso@stanford.edu

Model improvement by conditioning on data collected at multiple scales remains a challenge in complex settings. We employ an information-theoretic approach that allows for seamless integration of multi-resolution data into multi-scale simulations to upscale conductivity of heterogeneous formations. Fine-scale information is summarized into a coarse scale representation by setting a probabilistic equivalence between the fine and the coarse scale, with parameters that are determined via minimization of observables error and mutual information across scales.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-H / 516

Integrated Compositional Simulation and Optimization for Gas Mobility Control Techniques during CO2 Sequestration in Cranfield

Xueying Lu¹; Mohammad Lotfollahi²; Benjamin Ganis³; Baehyun Min³; Mary Wheeler³

¹ UT Austin
² The University of Texas at Austin
³ EWHA WOMANS UNIVERSITY

Corresponding Author(s): xylu@utexas.edu

CO2 sequestration in subsurface often suffers from poor volumetric sweep efficiency due to low gas viscosity, low gas density, and formation heterogeneity. This study aims to investigate CO2 mobility control techniques of Water Alternating Gas (WAG) and Surfactant (or Nanoparticle) Alternating Gas (SAG) to increase CO2 storage capacity in Cranfield Field, Mississippi via field-scale simulations and characterize key parameters critical to long-term CO2 storage success through optimizations. A parallel compositional simulator (IPARS) is used to accurately capture the underlying physical processes, with a field scale numerical model, over the desired time-span. A hysteretic relative permeability model enables modeling local capillary trapping. Foam-assisted CO2 mobility control technique is examined with an implicit texture foam model to investigate the eminent level of CO2 capillary trapping. A multipoint flux mixed finite element (MFMFE) method is used for spatial
discretization of the compositional flow model. It can handle complex reservoir geometries using general distorted hexahedral grid elements, as well as satisfy local mass conservation and compute accurate phase fluxes. The WAG and foam injection process are further optimized for injection bottom hole pressure, number of cycles, length of the cycles, and foam properties via GA (genetic algorithm) in UT optimization toolbox. Field scale simulations indicate that CO2 storage volume increases by 15% and 24% compared to continuous CO2 injection during WAG and foam processes, respectively. During SAG process, foam is generated in the high permeability streaks and upper layers with higher CO2 flow rates and diverts the CO2 flow into low permeability regions and bottom layers, leading to more efficient areal and vertical sweep efficiency. The optimized foam process saved 60% water and surfactant consumption comparing to the base case foam process while achieving same CO2 storage volume.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-G / 614

Integration of Pressure Transient Data into Reservoir Models using the Fast Marching Method

CHEN LI1, MICHAEL KING1

1 Texas A&M University-College Station

Corresponding Author(s): francis.chen.lee@gmail.com

Calibration of reservoir model characteristics by integration of well test data remains an important research topic. Traditional approaches to well test interpretation have relied upon simple homogeneous reservoir models, while the industry’s ability to develop more detailed and more heterogeneous static reservoir models has increased significantly. Pressure and rate data recorded at production (or injection) wells is readily available and can provide additional dynamic conditioning of these static models. Well test data has been recognized as an effective tool that can be used to describe transient flow behavior in petroleum reservoirs. It is also closely related to the drainage volume of the well and the pressure “front” propagation in the subsurface. Traditional analytic means of estimating reservoir permeability relies on an interpretation of the diagnostic plot of the well pressure and production data, which usually leads to a bulk average estimation of the reservoir permeability. Typical pressure interference tests involve injecting or producing fluid from one well while the pressure is recorded in another or more observational wells, where well pressure response can be affected by both geometry and flow regimes of the reservoir. Although only applicable to idealized models, the analytic approach provides the simplest methodology to obtain reservoir parameters through analysis of pressure changes. When more detailed characterization of reservoir heterogeneity is needed, a numerical inversion technique is required to integrate the observational data into reservoir models. Inverse methods for reservoir parameter estimation during history matching rely on establishing a robust forward model and then determining an objective function to be minimized. Generation of sensitivity coefficients for reservoir properties in all grid cells of the model is required, which becomes quite expensive as the model grows to a large size.

We utilize the concept of the “diffusive time of flight” (DTOF) to formulate an asymptotic solution to the diffusivity equation that describes transient flow behavior in petroleum reservoirs. The DTOF reduces the three-dimensional diffusivity equation to an equivalent one-dimensional form and is calculated by solving the Eikonal equation via the Fast Marching Method (FMM). Our method is tested on a two-dimensional synthetic heterogeneous reservoir model and applied to the three-dimensional Brugge field, where a single well with constant flow rate is simulated. The well test derivative is shown to be inversely proportional to the drainage volume and is treated as the objective function for inversion. Its sensitivity coefficients to the reservoir parameters are formulated analytically by taking the functional derivative of the Eikonal equation. The major advantage of formulating sensitivity coefficients using the FMM is its great computational efficiency while inversion is conducted, which is three orders of magnitude higher than numerical perturbation. With an additional constraint to honor the initial model, our inverse modeling approach will adjust the reservoir model to
obtain permeability as a function of distance from the well within the drainage volume. It provides a modification of reservoir permeability both within and beyond the “depth of investigation”.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 397

Interaction of pentane and 2-pentanone with UiO-66(Zr) by solid-state NMR

Marc Wagemann1; Bernhard Blümich1; Alina Adams1

1 ITMC RWTH University

Corresponding Author(s): wagemann@itmc.rwth-aachen.de

Metal organic frameworks (MOFs) consist of metal oxide cores linked by multifunctional organic linkers, forming crystal-like structures with well-defined pore size. They are highly promising materials in a large variety of applications including gas storage, solvent separation, drug delivery, and catalysis. The guest-host interaction is of key importance for all these applications and therefore its detailed understanding is fundamental for designing efficient MOF materials. This work investigates and compares for the first time the interaction of C5 alkane and ketone in a representative MOF material, the UiO-66(Zr), at ambient temperature by solid-state NMR. NMR methods have been already successfully applied to the study of structure, dynamics, and flexibility of different MOFs but they have been employed up to date only in very few cases for characterizing their interaction with liquid organic compounds largely at small loadings.

Pentane and 2-pentanone were chosen to represent C5 alkane and ketone. Both molecules are comparable in size, yet contain different functional groups and therefore are expected to have different interactions with the MOF materials. Furthermore, the guest-host interaction can be impacted by the structure of the MOF itself. In particular, UiO-66 is composed of smaller tetrahedral pores and larger octahedral pores. The adsorbent–adsorbate interaction was investigated in detail by a combination of 1H and 13C NMR MAS spectroscopy, 1H 2D NOESY experiments, and 1H site-selective relaxometry. Moreover, various solvent concentrations corresponding to different amounts of solvent molecules per MOF unit cell were also studied.

The obtained results show that the interaction of pentane with UiO-66 is strongly concentration dependent. At very low concentrations the pentane signals are shifted to positions towards lower ppm values with respect to the positions of the signals of the free pentane. The peak to peak distances between two nearby signals are decreased compared to the corresponding distances in the free pentane. With increased pentane concentration above a well-defined amount, the appearance of a second and then a third pentane species is observed. Both species have signals at the same chemical shifts as that of free pentane. Supported by numerical analysis, relaxometry results, and computational simulation, our data indicate that pentane can be found at low concentrations only in the smaller tetrahedral pores. With increasing concentration, the pentane molecules start to occupy also the larger octahedral pores and later on the inter-grain space. To our knowledge, this is the first time that three different types of solvent species are observed in a MOF material. The findings for pentane are compared to the results for 2-pentanone. In particular it was found that the peak to peak distance between two nearby signals for the first species is changed in such a way that only three signals are observable instead of the usual four. These findings contribute to a understanding of the adsorption mechanisms of small alkane and ketone molecules inside MOF pores.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 903
Interfacial Impacts on Slickwater Imbibition and Gas Production in the Marcellus Shale

Andres Clarens¹ ; Rodney Wilkins¹ ; Michael Plamprin²

¹ University of Virginia
² U.S. Geological Survey

Corresponding Author(s): andres@virginia.edu

Development in the dry unconventional gas-bearing Marcellus Shale in the Eastern United States has grown rapidly over the past decade. When a well is fractured in the Marcellus, only a small proportion of the slickwater fracturing fluid, typically <10%, is produced back following well completion. Most analyses also suggest that existing fracking and production practices only produce a fraction, typically <25%, of the Original Gas in Place (OGIP) over the life of the well. The connection between slickwater fate and gas production is poorly understood but it is generally assumed to involve trapping of imbibed water due to high capillary pressures, which impacts mobility of natural gas.

This work seeks to understand the connection between slickwater fluid properties, shale mineralogy and pore structure, and gas migration through fractured shales. Experiments were carried out to measure the fluid contact angles of Marcellus Shale mineral surfaces, representative fracturing fluids, and high pressure methane and the interfacial tension between fluids. These interfacial data were then integrated into a modeling framework developed using the EOS7C-ECBM equation of state modules within the TOUGH2 code, which includes the effect of non-Darcy flow regimes and sorption.

Our experimental results suggest that pre-wetted shale surfaces have a significantly lower static contact angle in the methane-water-shale system. Advancing contact angle on dry shale and drainage with receding angle on wet shale resulted in a difference of 70 degrees, illustrating the potential contribution of interfacial properties to relative permeability (Kr) and capillary pressure (Pc) hysteresis during imbibition and drainage in shale systems. These effects were correlated to specific Total Organic Carbon (TOC) content in the mineral. The experimental data were used to create synthetic inputs for using in the TOUGH2 code and the model was run to simulate flow behavior through the shale matrix, which was then used to represent different well configurations. Historical data of slickwater use and gas production from representative wells in the Marcellus region were used to benchmark the modeling output. The results suggest that there are key ways in which slickwater chemistry might be manipulated to increase the ultimate recovery of natural gas.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 667

Interfacial Processes Control Microbial Contamination and Cleaning of Fresh Produce

Yan Jin¹ ; Taozhu Sun¹ ; Anna Jurusik¹ ; Volha Lazouskaya²

¹ University of Delaware

Corresponding Author(s): yjin@udel.edu

Foodborne illnesses involving fresh produce have been increasingly causing concerns around the world. Pathogenic bacteria can attach to and colonize the surfaces of fresh produce, leading to contamination and illness outbreaks. However, mechanistic interactions between produce surface properties (e.g., roughness, topography and hydrophobicity) and bacterial retention remain poorly understood. As a result, effective strategies eliminating pathogenic contaminants for fresh produce
are not yet available. Using produce surfaces and their replicas, we systematically evaluated bacterial/colloid retention and removal as a function of physicochemical properties (roughness and hydrophobicity) of these surfaces as well as characteristics of water retention and distribution on the surfaces. We found that water retention and associated interfacial behavior associated with water on produce/replica surfaces are the key parameters that dominantly affect bacterial/colloid retention and removal, and those parameters in turn are collectively governed by surface roughness, topography and hydrophobicity. Based on these insights, we are developing new methods/strategies for more effective cleaning of fresh produce and other contaminated surfaces.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 971

Interfacial curvature and capillary pressure measurements during water displacement by supercritical CO2 in a micromodel

Farzan Kazemifar\textsuperscript{1} ; Yaofa Li\textsuperscript{2} ; Ava Hurlock\textsuperscript{3} ; Gianluca Blois\textsuperscript{2} ; Kenneth Christensen\textsuperscript{2}

\begin{itemize}
  \item \textsuperscript{1} California State University Sacramento
  \item \textsuperscript{2} University of Notre Dame
  \item \textsuperscript{3} University of Rochester
\end{itemize}

Corresponding Author(s): farzakazemifar@csus.edu

Multiphase immiscible displacement in porous media is a process occurring in different applications, such as CO2 sequestration in saline aquifers and oil/gas production from hydrocarbon reservoirs. Capillary pressure, \(P_c\), is one of the variables that controls flow behavior and displacement patterns that ultimately determines residual saturation. Capillary pressure is a function of interfacial tension and interfacial curvature. In this work, displacement of water by supercritical CO2 in a heterogeneous micromodel is studied using a high-speed camera coupled to a long-distance microscope with large field of view. Interfacial curvature of individual menisci is measured to estimate the capillary pressure in each meniscus. The correlation between the dynamic local capillary pressure measurements and pressure difference across the micromodel during the drainage process is examined in detail.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 266

Investigating Capillary Pressure Behavior in Mudrocks through Grain Scale Modeling

Author(s): Abhishek Bihani\textsuperscript{1}
Co-author(s): Hugh Daigle \textsuperscript{1}

\begin{itemize}
  \item \textsuperscript{1} The University of Texas at Austin
\end{itemize}

Corresponding Author(s): abihani@utexas.edu
The capillary entry pressure (Pce) and corresponding pore throat size control the thickness of an oil or gas column that may be sealed beneath a mudrock. Mudrock seals typically have nanometer-scale pore throats, and the Pce often exceeds the minimum horizontal effective stress in these rocks. Mudrock seals can fail through fracturing either by buildup of fluid pressure or during faulting or folding, creating fractures with much smaller Pce than the pore space, allowing hydrocarbon to escape. Understanding the factors at the grain and pore scale that influence Pce is an important component of risk assessment and prospect evaluation.

Prediction of capillary pressure and relative permeability behavior is especially difficult in shaly sands and mudrocks as the sediments are usually heterogeneous mixtures made of disparate grains shapes and sizes. Mudrocks are primarily a mixture composed of silt (coarse) and clay (fine) grains. The porosity for a mudrock varies according to the fractions of these components, and the minimum porosity is achieved when clay particles occupy all the interstitial space between the larger silt particles (Daigle and Reece, 2014). Schneider et al. (2011) showed that silt bridging, in which silt-sized grains are present in an abundance sufficient to create a connected stress chain through the rock matrix, preserves large pore throats, thereby affecting the permeability as well as Pce.

To simulate these effects at grain scale, bidisperse sphere packs were generated by a cooperative rearrangement algorithm for efficient packing with the ratio of larger to smaller spheres as 5:1. We varied the different sphere volume fractions to mimic mudrocks. The generated sphere packs were subsequently converted to pore throat models by employing Delaunay tessellation similar to Mehmami and Prodanovic (2014). Following Mason and Mellor’s (1995) approach, an invasion percolation algorithm was applied to the models to generate drainage and imbibition capillary pressure curves and relative permeability curves.

It was observed that on successive increase of the fraction of larger spheres in a sphere pack, the capillary pressure curves displayed a dual percolation threshold behavior. This can be explained by larger pores being preserved adjacent to the spheres due to the silt-bridging effect as implied by Schneider (2011). These larger pores are responsible for the lower percolation threshold, while smaller pores between smaller grains give rise to the higher capillary threshold. Increasing the larger sphere fraction also decreased the residual water phase saturation, possibly due to the trapped phase escaping through the larger pores. This confirmed that the concentration and radius-ratio of the grains strongly affect the capillary pressure behavior in dual-component systems like mudrocks.

The next step in this project will be exploring the capillary behavior at different sphere-radius ratios and distributions, and for sphere packs generated by sequential addition under the effect of gravity. The principal application of this work is improved assessment of seal capacity from microstructural data in deep-water, subsalt environments. Ultimately this work may affect estimates of reserve capacity of reservoirs and risk management efforts in developing prospects by providing a more accurate understanding of seal quality.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-C / 541

Investigating the influence of aperture variability on fracture surface area in enhanced geothermal reservoirs

Philipp Schädle1 ; Anozie Ebibo2 ; Martin O. Saar3
To estimate the performance and sustainability of enhanced geothermal systems (EGS), an accurate characterization of the fractures created by hydraulic stimulation is crucial. It is common practice to perform tracer tests to obtain relevant reservoir parameters such as reservoir impedance, potential production flow rate as well as fracture surface area [Shook, 2017]. The fracture surface area is one of the most relevant parameters for heat transfer between the rock and the working fluid. However, it is also one of the most uncertain parameters in the characterization of fractured reservoirs. Generally, fractures of all scales are characterized by two opposite rock surfaces with variable surface roughness. Consequences of varying surface roughness are a heterogeneous local aperture distribution and the formation of channels and barriers within the fracture planes. This significantly affects flow and transport and the resulting fracture surface area. In summary a heterogeneous local aperture distribution is highly relevant for heat extraction. In a typical rock fracture, the local aperture is statistically represented by a spatially autocorrelated random field, which is characterized by the variogram model and a correlation length [Tsang, 1989].

In this study, we investigate the influence of correlation length with respect to aperture distribution on fracture surface area and its implication for the results of tracer tests. To this end, numerical simulations of a single circular fracture embedded in a low permeability host rock are performed. Various heterogeneous aperture fields with different correlation lengths are considered. Using a mixed-dimensional discretization to represent the fracture numerically allows us to model heterogeneous fractures by applying the corresponding material parameters. In the fracture plane, flow and tracer transport occurs between an injection and a production well. The numerically calculated fracture surface area is compared to the results of analytical methods where the fracture surface area is calculated based on the injected and produced tracer rates [Shook, 2017]. Furthermore, our simulations enable the investigation of the influence of different correlation lengths on the results of tracer tests. We show how the aperture variability impacts the results of tracer tests and the fractured surface area. Our results contribute to improvement of reservoir characterization and performance assessment of EGS.

References:
Click here to agree

Poster 3 / 813

Investigation of Radial Capillary Penetration Kinetics in Virtual 3-D Porous Media Using Direct Numerical Simulations with Volume-Of-Fluid Method

An Fu¹ ; Nikhil Palakurthi² ; Ken Comer² ; Milind Jog³

¹ PhD Student
² Procter & Gamble
³ University of Cincinnati

Corresponding Author(s): fuan@mail.uc.edu
Capillary flow penetration can be categorized into two directions: Unidirectional (Linear) and Radial. The fluid invasion physics has been extensively studied for linear flow direction. Danino & Marmur study radial capillary penetration in a filter paper experimentally, and the results indicate a power-law correlation between average wicking radius and time. It shows the average spreading radius follows $R \sim t^{0.425-0.44}$. And this wicking kinetic is slower than linear regime where $L \sim t^{0.5}$. The first goal of this research is to answer the question that why radial capillarity is slower than linear penetration. Another main purpose is to investigate the influence of pore connection and mean pore radii on the macroscopic capillary radial spreading. Direct Numerical Simulations (DNS) using Volume-Of-Fluid (VOF) method will be performed using an open source code OpenFOAM; gravity is ignored in the simulations due to its negligible influence. Important variables which include wicking radius, capillary pressure and inlet velocity will be analyzed.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-E / 99

Investigation of two-phase flow in a new pore doublet model

Lei Zhang$^1$; Pengfei Liu$^1$; Jun Yao$^1$

$^1$ China University of Petroleum

Corresponding Author(s): zhlei.upc@gmail.com

Pore-scale flow modeling based on pore network model is an efficient simulation method. However, the distribution of two-phase fluid in pores and throats is based on the two-phase numerical simulation results in a single channel during the simulation of two-phase flow. The influence of pore-throat topology and pore-throat ratio cannot be considered. Hence, a new pore doublet model is proposed, named pore-throat doublet model. Only two kinds of flow behaviors can be observed in conventional parallel dual-channel model: single-channel intrusion and dual-channel simultaneous intrusion. However, a new flow behavior, slug flow, was found in the simulation of two-phase flow in the new pore doublet model, which could not be observed in the conventional model. Finally, a series of researches on slug flow were carried out. The range of conditions for slug flow formation was obtained by considering different channel width ratio, Ca number and different pressure drop.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 1-F / 950

Is Ostwald Ripening Important in CO2 Geological Sequestration? A Micromodel Study of Bubble Repining Dynamics

Author(s): Ke Xu$^1$; Matthew Balhoff$^2$

Co-author(s): Roger Bonnecaze$^2$

$^1$ University of Texas at Austin

$^2$ McKetta Department of Chemical Engineering and Texas Materials Institute, The University of Texas at Austin
Corresponding Author(s): thnk-xu08@utexas.edu

- Theoretical part of this work has just been accepted by Physical Review Letters

Long-term storage is necessary in order for CO2 geological sequestration in to be feasible. Leakage of CO2 by buoyant forces may occur if the trapping of CO2 in porous media is not stable with formation of large CO2 clusters. Ostwald ripening is a well-known phenomenon in two-phase mixtures that may affect bubbles’ stability. During an Ostwald ripening process in an open system, the gas in small bubbles dissolves in the surrounding fluid and diffuses to larger bubbles to grow them. Thus, there is concern about whether a coarsening of CO2 bubbles can occur and lead to such leakage after injection into porous media.

Here we show that Ostwald ripening will not lead to considerable coarsening of CO2 bubbles trapped in porous media. The size evolution of bubbles in a micron-scale porous medium has been shown very different from that in an open system. Unlike the coarsening typically observed in open systems, an initially polydisperse population of bubbles will ultimately become monodisperse and there is egalitarianism in bubble size for sufficient confinement in a homogenous porous medium, with gas from the larger bubbles diffusing to smaller bubbles.

Experiments conducted on a 2.5-D micromodel validate the ripening dynamics models, with the bubble population evolution dynamics well quantified. Our results show that this anti-coarsening effect is driven by the capillary pressure difference, and directed by the micron-scale geometric confinement. A physical model for the evolution dynamics on bubble population is derived from first principles with no empirical parameters, and this model matches our experimental data very well.

Based on our experiments and models, we conclude that, Ostwald ripening can be a positive effect, rather than a negative effect, to improve bubble stability. If bubbles are initially dispersed into small size (similar to or smaller than pore size) during injection, no significant coarsening will happen that lead to gas leakage. In addition, understanding this anti-coarsening effect of bubbles/droplets in porous media is also of great significance for better description and operations in many other applications which involve time scales similar to or longer than several hours, such as the formation and concentration of oil and gas in reservoirs (millions of years), transport of NAPLs in soil (days or even years), foam-based enhanced oil recovery (months to years).

References:

Ke Xu, Roger Bonnecaze, Matthew Balhoff. “Egalitarianism among bubbles in porous media: An Ostwald ripening derived anti-coarsening phenomenon”, Physical Review Letters, just accepted Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 958

Joint stochastic modeling using copulas for the dependency between petrophysical properties and seismic attributes at well-logs scale

Author(s): Daniel Vázquez Ramírez

Co-author(s): Martin Díaz-Viera ²; Huong Le Van ³

¹ Institute of Geophysics, UNAM
² Mexican Petroleum Institute
³ Institute of Geophysics

Corresponding Author(s): mdiazv@imp.mx

The use of petrophysical data and seismic attributes in the oil industry have allowed the characterization of the reservoirs due to their value as predictive tools, for the evaluation of reservoir information is needed the petrophysical parameters such as porosity, permeability, saturation, etc. And the seismic information can infer the physical properties of the rocks on the place (Li & Zhao, 2014).
However, we have problems related to the characterization of these reservoirs due to the uncertainty inherent in the data, in most of the studies conducted in earth sciences is fragmented, we have limited information, it is not statistically representative, or you must resort to nonparametric perspectives to reduce the error in the calculations based on the data obtained and thus, comply with the aspect of continuity.

Due to this condition, stochastic modeling is used, which is an effective tool that allows obtaining the probability distribution of one or several random variables, in this case of the petrophysical data and seismic attributes, so we can manage the uncertainty of the generated model, especially if the spatial distribution is not so good.

Recent work has modeled the dependency relationship between seismic attributes and petrophysical properties using Geostatistical estimation methods such as Cokriging (J.O. Parra, Iturrarán-Viveros, Parra, Jiménez-Andrade, & Carrillo-Calvet, 2015), (J. Parra & Emery, 2013). This approach requires that the model has a strong “linear” dependence between the properties because otherwise their application is not viable, which is uncommon in deposits with complex lithologies. On the other hand, estimation methods such as Cokriging underestimate the dispersions and extreme values that exist in the data, which can be critical for properties such as permeability, where the most important are high values (preferential flow paths) or very low (seals). As alternative can be used stochastic model with general dependences using copulas (Diaz-Viera, et al, 2016).

A copula is a set of functions that combine or couple the function of multivariate distribution with their marginal distribution functions and whose marginal distribution function is uniform (Nelsen, 1999). Then, we can represent the dependency structures between one or several petrophysical properties with one or several seismic attributes, this represents a very important advantage, since for the copulas it is not required that the dependence between the petrophysical properties and seismic attributes be of some type specific (Diaz-Viera, Erdely, Kerdan, del-Valle-Garcia, & Mendoza-Torres, 2017).

The application of the method is shown in a case study of deep marine reservoir at well-log scale.

References:

Click here to agree

**Parallel 5-B / 648**

**Kerogen flexibility, a key to understand hydrocarbon expulsion from shale reservoirs?**

Amaël Obliger†; Pierre-Louis Valdenaire†; Nicolas Capit†; Franz-Josef Ulmi†; Pellenq Roland†; Jean-Marc Leyssale†

† Massachusetts Institute of Technology, MSE2 MIT-CNRS International Joint Unit
Corresponding Author(s): plvalden@mit.edu

A common assumption in recent molecular simulation based investigations of hydrocarbon transport in kerogen is that the latter behaves as a rigid matrix [1-4]. In other words, its porosity remains relatively constant and irrespective of temperature, lithostatic (or external) pressure or fluid (or adsorption) pressure. This implies that the matrix isolates the fluid from external pressure effects and that, diffusion and transport are only affected by the free pore volume, a lower amount of adsorbed fluid implies a higher amount of free volume and thus a higher diffusion coefficient [3]. However, it was shown that, immature kerogen, in particular, can retain a high (soft) aliphatic content and present low stiffness [5], typical of compressible media. Here we use an amorphous hydrogenated carbon model with high aliphatic content as a proxy for immature kerogen and characterize its poroelastic behavior in large ranges of temperature, lithostatic pressure and fluid pressure and determine the sorption isotherms of methane accounting for swelling. Results show that the pore space depends considerably on the three parameters and that the matrix behaves as an ideal adsorbent (linear increase of sorbate amount with the fluid pressure) up to very high pressures due to considerable swelling. An important consequence of swelling is that instead of decreasing with loading as is the case in rigid frameworks, the self diffusion coefficient of methane actually increases with loading. Furthermore, simulation of methane desorption at kerogen/macropore interfaces reproduces the well-known productivity decline of shale-oil plants when matrix flexibility is accounted for while the conventional fikkian regime is obtained in the rigid approximation. We associate this anomalous transport phenomenon to a macroscopic deformation of the matrix taking place during fluid desorption.


References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-G / 631

LBM study of non-isothermal liquid evaporation in specifically designed porous media

Feifei Qin¹ ; Luca Del Carro² ; Ali Mazloom Moqaddam³ ; Qinjun Kang⁴ ; Dominique Derome⁵ ; Jan Carmeliet⁵

¹ ETHZ/Empa
² IBM-Zurich
³ Empa
⁴ Los Alamos National Laboratory
⁵ ETH Zurich

Corresponding Author(s): feifei.qin@empa.ch

Liquid evaporation rate in porous media is often characterized by two distinct periods. A first drying period (stage I) is characterized by a relatively high and constant drying rate referred to as constant rate period (CRP) where evaporation is supported by a fast internal capillary flow and controlled by the boundary conditions. The second drying period (stage II) is characterized by a lower and gradually dropping evaporation rate also termed falling rate period, FRP, due to the transition to
diffusion-limited vapor transport. We study here stage I evaporation for specifically designed porous media both numerically and experimentally with the aim to control their drying rate. We conduct evaporation experiments with quasi-two-dimensional microfluidic porous systems and model the behavior with a lattice Boltzmann model tailored to the specific needs of such phenomena. A hybrid thermal entropic multiple-relaxation-time multilange pseudopotential lattice Boltzmann model (EMRT-MP LBM) is applied to simulate the non-isothermal liquid-vapor phase change during evaporation and provide the exact water configuration within complex porous media. First this model is validated by comparing with the diameter square law for a single droplet evaporating in a closed cavity. Then liquid evaporation in spiral-shaped and gradient-shaped micro-pillared cavities, referred as SMC and GMC, is studied. For the experiments, microfluidic systems measuring 5 x 5 mm² are imaged with fluorescent microscopy, under controlled boundary conditions. Both simulation and experiment results show that in SMC the evaporation route follows the spiral shape, while in GMC the liquid evaporates layer by layer, i.e. from large pore rows to small pore rows. The explanation of the phenomenon is that, since the surrounding vapor pressure is almost constant, the liquid pressure at liquid-vapor interface with larger radius is higher due to surface tension effects. Thus liquid will flow from the large-radius menisci to the small-radius menisci between pillars due to the difference in liquid pressure. As a consequence, the evaporation front at the larger interface will move first while the interfaces at the smaller pillar distance will remain longer in place. The evaporation rate reduces slightly with time due to the decrease of the liquid-vapor interfacial area. Both the simulation and experiment results show that stage I liquid evaporation may occur in well-designed porous media for long time.

References:
1 Feifei Qin, Ali Mazloom Moqaddam, Qinjun Kang, Dominique Derome, Jan Carmeliet. (2017) Entropic multiple-relaxation-time multilange pseudopotential lattice Boltzmann model for two-phase flow; Physics of Fluids, under review. Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 261

Laboratory Investigation of Liquid Injectivity in Surfactant-Alternating-Gas Foam Enhanced Oil Recovery

JIAKUN GONG1 ; Sebastien Vincent-Bonnieux2 ; Ridhwan Zhafri Kamarul Bahrim3 ; Jeroen Groenenboom2 ; Rouhi Farajzadeh4 ; William Rossen2 ; Rodrigo Orlando Salazar Castillo4

1 Delft University of Technology
2 Shell Global Solutions International
3 PETRONAS
4 TU Delft

Corresponding Author(s): r.o.salazar@tudelft.nl

Foam can improve sweep efficiency in gas-injection enhanced oil recovery. Surfactant-alternating-gas (SAG) is a favored method of injection, in part because of excellent injectivity during gas injection. However, liquid injectivity is usually very poor in a SAG process, and fracturing of the well can occur. We report a coreflow study of liquid mobility under conditions like those near an injection well in SAG application in the field: i.e., after a prolonged period of gas injection following foam. We inject foam, gas (nitrogen) and surfactant solution into a 17-cm-long Berea core at elevated temperature (90 °C) with 40 bar back-pressure to minimize gas-expansion effects. Pressure differences are measured separately across five sections of the core and supplemented with CT scans to relate water saturation to mobilities. From these data we estimate the velocities, saturation changes, and mobilities of the various banks that determine liquid injectivity. We examine liquid injection directly following a period of foam injection, as in previous studies, and then following prolonged periods of gas injection following foam, to reflect injectivity near the well in a SAG process. Liquid injectivity directly following foam is very poor, as shown in previous studies. Liquid first fingers through the trapped foam. It then dissolves gas trapped within the liquid fingers, and the overall mobility rises sharply. During prolonged gas injection following foam, however, a region forms near the inlet and slowly propagates downstream in which gas mobility is much greater. The abrupt rise
in gas mobility appears to reflect the decline in water saturation below about 0.2 in our experiments. This decline in liquid saturation reflects in part liquid evaporation, and also pressure-driven flow and capillary effects on the core scale. In the region of lower liquid saturation, subsequent liquid mobility is much greater than downstream, and liquid sweeps the entire core cross-section rather than a single finger. Mobility in the region of liquid fingering is insensitive to the quality of foam injected before gas and the duration of the period of gas injection. These results suggest that there is a small region very near the well, crucial to overall injectivity, in which liquid mobility is much greater than that further from the well. These conditions are not described by current foam models. The results can inform a model for liquid injectivity based on radial propagation of the various banks seen in the experiments.

References:

Poster 1 / 605

Laboratory investigations of geochemical evolution in unconventional reservoirs during hydraulic stimulation

Johnathan Moore$^{1}$, Alexandra Hakala$^{2}$, Christina Lopano$^{3}$, Dustin Crandall$^{4}$, Sarah Brown$^{5}$, Thai Phan$^{6}$, Wei Xiong$^{6}$

$^{1}$ AECOM, National Energy Technology Laboratory
$^{2}$ NETL
$^{3}$ National Energy Technology Laboratory
$^{4}$ U.S. Department of Energy National Energy Technology Laboratory
$^{5}$ AECOM, contractor for NETL
$^{6}$ Oak Ridge Institute for Science and Education at the National Energy Technology Laboratory

Corresponding Author(s):

Hydraulic fracturing fluids (HFF’s) have been used for several decades to control mechanical, hydraulic, and geochemical behavior in unconventional reservoirs during stimulation. The interactions that occur in these environments during stimulation (hydrofracturing) are designed to prevent scaling, improve production, and prevent damage to formations. However, there is still uncertainty with regards to near fracture geochemical reactions and the evolution of the fluids temporally as they interact with the reservoir rock.$^{1}$

Rock cores taken from the Marcellus shale, both in outcrop and from a production well, were exposed to simulated HFF’s and simulated formation brines (SFB). The fluids were designed based on regional averages obtained from operators. The tests were conducted at pressures and temperatures representative of regional reservoir conditions, 19.3 MPa and 71°C respectively, and with all fluids under a nitrogen atmosphere to limit free oxygen. Core samples were fractured and loaded with 40/70 US Silica White™ quartz proppant. Tests lasted approximately 96 hours with low flow rates to represent a shut-in period. Geochemical samples were taken daily and analyzed using Inductively Coupled Plasma Mass Spectrometry and Ion-Chromatography. Imaging of the cores was done before exposure using Computed Tomography (CT) scanning and after exposure using CT, Scanning Electron Microscopy (SEM), and Raman Spectrometry.

Control samples, using deionized water as the flow medium, exhibited little to no change in the rock core or in the effluent of the system, dominated by Ca and SO4. Experiments using only SFB showed minor increases in major elemental chemistry in the effluent, consistent with minor dissolution or entrainment of free particles, and minor precipitation of barite/calcite on the fracture surface observed with SEM. HFF chemicals, without SFB, resulted in increases in most elemental constituents in the effluent, with few exceptions including barium which showed an increase followed by a major decrease in concentration. The rock core exhibited significant reaction in CT images and only minor traces of barite/calcite precipitation. The combination of HFF and SFB resulted in large increases in most metal constituents in the effluent during the reaction with the core and significant alteration of the rock matrix adjacent to the fracture. However, this mixture resulted a continual decrease in Ba and SO4 during the experiment, signaling potential deposition of these constituents.
In general, experiments indicated minor pyrite oxidation/dissolution, dissolution of carbonates, and minor precipitation of barite. The degree of precipitation was not of the magnitude observed in Paukert et al. (2017), but there is evidence that carrier fluid composition (~90% of the total volume) is an important consideration in precipitation within unconventional systems and may provide the nucleation surfaces for precipitation. Work continues analyzing precipitates, fracture surfaces, and base-fluid importance in precipitation.

References:

Click here to agree

Parallel 9-G / 17

**Lagrangian transport and chaotic advection in a class of (anisotropic) subsurface reservoirs**

Michel Speetjens¹; Stephen Varghese¹; Ruben Trieling¹

¹ Eindhoven University of Technology

**Corresponding Author(s):** m.f.m.speetjens@tue.nl

Subsurface scalar transport of e.g. heat or chemicals by fluid flow is key to problems as enhanced oil recovery, enhanced geothermal systems, carbon sequestration or in situ minerals mining. The Lagrangian transport properties of the subsurface flow are crucial in such processes. For example, recent studies in the literature on a two-dimensional (2D) unsteady Darcy flow in a circular reservoir driven by reoriented injection–extraction wells demonstrated that well configurations and pumping schemes designed via chaos theory enable efficient fluid distribution (for e.g. in situ mining) through the entire reservoir. Central to this is accomplishment of chaotic advection, i.e. the rapid dispersion and stretching of material fluid elements, by "proper" flow forcing. Problems as e.g. groundwater remediation may, on the other hand, require targeted delivery (and subsequent confinement) of fluid containing chemicals to designated regions of the reservoir for local contaminant treatment. This may be achieved by systematic creation and manipulation of Lagrangian transport barriers.

The present study seeks to deepen insight into generic subsurface Lagrangian transport by investigating the formation of so-called Lagrangian coherent structures (LCSs) as e.g. the above transport barriers as well as the accomplishment of (localised) chaotic advection. To this end theoretical and computational analyses are performed for the above 2D circular reservoir. This reveals that, in general, appropriate pumping schemes enable systematic and robust creation of various Lagrangian transport conditions for given well configurations (e.g. confinement zones of controlled size embedded in a chaotic environment). A key aspect is the impact of anisotropy in the porous matrix. Such anisotropy generically eliminates key organizing mechanisms, viz. symmetries, and thus tends to promote disorder and, inherently, chaotic advection at the expense of LCSs. However, symmetries are partially preserved — and thus order and coherence partially restored — for certain pumping schemes and well configurations aligned with the anisotropy. Symmetry associated with well alignment in fact gives rise to an intriguing “order within chaos” observed only in such cases: prolonged confinement of fluid to subregions of chaotic areas.

References:

**Acceptance of Terms and Conditions:**

Click here to agree
Lattice Boltzmann Simulation of Liquid Flow in Nanoporous Media

Jianlin Zhao\textsuperscript{1} ; Qinjun Kang\textsuperscript{2} ; Jun Yao\textsuperscript{3} ; Lei Zhang\textsuperscript{4} ; Zheng Li\textsuperscript{3} ; Yongfei Yang\textsuperscript{4} ; Hai Sun\textsuperscript{5}

\textsuperscript{1} China University of Petroleum (East China)  
\textsuperscript{2} Los Alamos National Laboratory  
\textsuperscript{3} China University of Petroleum, Qingdao  
\textsuperscript{4} China University of Petroleum  
\textsuperscript{5} Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China), Qingdao, China

**Corresponding Author(s):** qkang@lanl.gov

A multi-relaxation-time lattice Boltzmann (LB) model for nanoscale liquid flow is developed to investigate the liquid flow characteristics in nanoporous media. The slip length and effective viscosity obtained from molecular dynamics (MD) simulations are adopted to account for the nanoscale effect. First, the LB model for water flow in nanopores is built and water flow characteristics in nanoporous media are investigated. The results show that: (1) the nanoscale effect can either increase or decrease the water flux in nanoporous media, depending on the solid-solid interaction force; (2) the nanoscale effect impacts the velocity distribution in porous media, making it more uniform in hydrophobic porous media while more heterogeneous in hydrophilic porous media; (3) the end effect caused by the bending of streamlines plays a significant role in water flow in nanoporous media, and neglecting the end effect can greatly overestimate liquid flow ability; and (4) the pore structure also has significant influence on water flow in nanoporous media. With the increase of specific interfacial length, the nanoscale effect increases. In addition, the LB model for oil (octane) flow in quartz nanopores is also established by incorporating the MD simulation results. Oil flow simulation in quartz nanoporous media shows that the conclusions obtained for water flow are also applicable for oil flow.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

Parallel 1-C / 982

Lessons learned in the North Sea: Closing the gaps in permanent well plugging

Malin Torsater\textsuperscript{1}

\textsuperscript{1} SINTEF

**Corresponding Author(s):** malin.torsater@sintef.no

All wells will one day need to be permanently plugged and abandoned (P&A’ed), and this last phase of a well’s life cycle does not end – but has an eternal perspective. The North Sea is a mature petroleum region, and a heavy focus on P&A activities are planned here for the next decades. Research and technology development needs to keep up with this shift in activity level, and a strong focus has thus recently been put on R&D relevant for P&A in Norway.

This talk will give an overview of P&A challenges and opportunities in the North Sea. First of all, it will point out exactly why today’s P&A operations are so time consuming and expensive. Technology gaps will be outlined, together with issues related to standards and regulations in the North Sea countries. Thereafter, emerging P&A solutions will be discussed, and results will be shared from ongoing R&D projects aiming to simplify future P&A operations. Examples of topics that will be outlined are:

- Making use of shale formations as permanent barriers in wells
- Techniques for simpler removal of steel pipes from wells
- Methods for avoiding steel removal during P&A
- Advice for maximizing long-term integrity of plugged wells
  Thoughts about possible value creation from P&A, which is an ever-growing and long-lasting market, will also be shared with the audience. Differences between the North Sea and the Gulf of Mexico when it comes to plugging costs and operations will also be outlined.

References:
Acceptance of Terms and Conditions:
Click here to agree

Invited 1 (Room B) - Hamdi Tchelepi / 1117

Level-set method for modeling pore-scale two-phase flow at small capillary numbers

Author(s): Hamdi Tchelepi
Co-author(s): Moataz Abu-Al-Saud

1 Stanford University

Corresponding Author(s): tchelepi@stanford.edu

We developed a sharp-interface level-set method for immiscible pore-scale two-phase flow with a thin wetting film on the solid surface. The lubrication approximation is used to model the thin-film equation efficiently. The incompressible Navier–Stokes, level-set, and thin-film evolution equations are coupled sequentially. Hamilton–Jacobi level-set reinitialization is employed to construct the signed-distance function, which takes into account the thin film on the solid surface. The level-set simulation method is validated and shown to match the augmented Young–Laplace equation for a meniscus in a capillary tube. Viscous bending of an advancing interface over a precursor film is captured by the level-set method and agrees with the Cox–Voinov theory. We model the evolution of an advancing bubble surrounded by a wetting film. The predicted film thickness compares well with both theory and experiments. We then demonstrate that the multiscale level-set approach can model immiscible two-phase flow with a capillary number as low as 10⁻⁶.

References:
Acceptance of Terms and Conditions:
Click here to agree

Invited 2 (Room B) - Ian Griffiths / 1114

Leveraging mathematics for global filtration challenges

LM. Griffiths

1 University of Oxford

Corresponding Author(s):

The Ganges–Brahmaputra Delta is a global hotspot for arsenic groundwater contamination. Naturally occurring arsenic concentrates in water drawn from deep wells, creating a major public health issue in West Bengal and Bangladesh that has been described as the largest mass poisoning of a population in history. A novel technology has recently been discovered that uses naturally abundant laterite soil to filter arsenic. This technology has the potential to provide a global breakthrough, supplying clean water to the world. However, to achieve this, a sound quantitative understanding of its behaviour is essential, which can only be obtained through the development of mathematical models.
In this talk we present a mathematical framework that uses homogenization theory to distil the complex process to a simple model. The resulting framework predicts how frequently filters must be replaced and how the filters may be upscaled to serve, for example, a school or community. The filter has been piloted in three communities in India, serving more than 5000 people, and the tools that we have developed will provide the essential guidance needed for engineers to maintain current filters and deploy these new filters in a cost-effective manner.

We will also outline how the framework is applicable to the wider filtration context of porosity-graded filters that offer superior filtration properties and improved blocking resistance.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-H / 112

Low Frequency Vibrations as the Indication of the Structural Transformations in Zeolitic Imidazole Frameworks – Density Functional Theory Study

Filip Formalik¹ ; Michael Fischer² ; Bogdan Kuchta³

¹ Group of Bioprocess and Biomedical Engineering, Faculty of Chemistry, Wrocław University of Science and Technology, Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wrocław University of Science and Technology

² Crystallography Group, Department of Geosciences, University of Bremen

³ Laboratorie MADIREL

Corresponding Author(s): filip.formalik@pwr.edu.pl

Low frequency lattice vibrations (<100 cm⁻²) are indicators of variety of structural transformations in the metal-organic frameworks (MOFs). In the case of zeolitic imidazole frameworks (ZIFs) ZIF-4, ZIF-7 and ZIF-8, the terahertz vibrations which are responsible for such phenomena as gate opening mechanism, shear-induced deformations or breathing. ZIFs are promising materials not only for the classical porous materials applications (CO₂ capture, separation of hydrocarbons) but also as possible hosts for catalytically active compound (nanoparticles), drug delivery or even as shock-wave mechanical absorbers.

We selected ZIF-8 as the precursory framework for our research. This well-known sodalite-type cage material allows introducing a variety of chemical and structural modifications. We defined three groups of ZIF-8-derivative materials with (i) different metal ions in metallic centers (B3⁺ and Li⁺ or Cu⁺ at the tetrahedrally coordinated positions - BIF-3 family, Co2⁺ - ZIF-67, Cd2⁺ - CdF-1), (ii) different functionalization of imidazolate ring (-H – SALEM-1, –NO₂, –H, –NH₂, –CHO – ZIF-90) and (iii) different geometry (ZIF-7 and ZIF-9 – Zn- and Co-based frameworks with benzimidazole as a linker and with elongated 6-meber ring). We used density-functional theory in conjunction with the finite displacement method to predict and visualize the normal modes (vibrations) of the lattice. The results allows us to determine how changes in composition or geometry affect the presence and frequency of the mode related to the gate opening mechanism. We show that there are several participating modes. The first one is a symmetric distortion of the framework leading to the opening of the pore (IR inactive due to its symmetry) and a collection of IR active modes which might lead to asymmetric gate-opening. We claim that the frequency of the IR inactive “gate opening” mode is determined by the interactions between the linkers, therefore depending on attraction/repulsion force competition in the attached functional groups. At the same time, the frequencies of the IR active modes are sensitive to the variation of the linker mass. Additionally, we show that the elongation of the M-N (M = metal ion) distance when Zn in ZIF-8 is substituted by heavy Cd ion leads to the shear deformation of the 4-meber ring. This corresponds to a mode at around 22 cm⁻¹ in the precursory ZIF.

In conclusion we show that the potential structural deformations (or transformations) which occur in zeolitic imidazole frameworks can be predicted from vibration in the low frequency phonon spectrum.
References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-D / 924

Low-Field Nuclear magnetic resonance characterization of Carbonate and Sandstone Reservoirs

Heng Wang¹ ; Vladimir Alvarado¹

¹ University of Wyoming

Corresponding Author(s): hwang19@uwyo.edu

Laboratory measurements, i.e. gas (N₂) porosity and permeability, time-domain nuclear magnetic resonance (NMR) including transverse relaxation time (T₂) and diffusion coefficient, and thin section and scanning electron microscopy (SEM) analysis, were conducted to obtain petrographical and petrophysical descriptions of the Weber Sandstone and Madison Limestone at the Rock Spring Uplift, a potential carbon dioxide site in Southwestern Wyoming. The relationships between pore structures, such as pore geometry, pore-size distribution, pore network, and porosity/permeability were investigated. First, using thin sections combined with electronic microscopy for the description of pore structures, all samples are described in detail from the geological, petrographical and diagenetic point of view. Results show that within the Madison Limestone pore systems, pore types include intercrystalline, vuggy, moldic, or mixed (combination of all other pore types). Both moldic and vuggy pore types are associated with samples of high porosity and permeability. NMR relaxation time distributions show either bimodal or multimodal distributions. Large relaxation time components are associated with samples with large pores, whereas small component are dominated by small pores. Permeabilities predicted by the log mean of T₂ shows a good correlation with gas permeability for Weber Sandstone samples. While for Madison Limestone samples, permeabilities predicted by NMR method are over- or underestimated when permeability is small due to pore coupling effect. In addition, short-time diffusion coefficients (D) were measured by pulsed field gradient (PFG) NMR method using a series of gradient strengths, and diffusion coefficient distributions were calculated. We found that diffusion coefficient distributions are consistant with the corresponding T₂ distributions for macropores. However, for micropores, diffusion coefficient peak vanished because of fluid-rock interaction and/or small value of brine saturated in. Furthermore, by comparing the dominant peak position of T₂ distributions and their corresponding diffusion coefficient distributions, we predicted the surface relaxivity of different rock types. We found that surface relaxivities of Weber Sandstone samples can be well predicted, while for Madison Limestone samples, surface relaxivities are overestimated due to diffusive pore coupling effect.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 824

MODELING OF LOW SALINITY WATERFLOODING THROUGH FRACTURED CORES

Carlos A. Romano-Pérez¹ ; MARTIN DIAZ-VIERA²
In this work a methodology is presented for modeling a fractured porous media and to simulate oil recovery by low salinity water injection through a fractured core. To represent the porous matrix a continuum approach is employed whereas for the fractures a discrete one. Thus, the fractured core is modeled with mixed dimensions elements, representing the fractures as elements of n−1 dimensions immersed in a porous matrix of n dimensions by isolated internal boundaries, where the equations that govern the flow of fluids in the matrix and the fractures are coupled by means of jump and average equations, taking into account interactions between the fractures and the surrounding porous media. The derived flow model in fractured porous media is bi-phasic, based on the saturation and total velocity. The effect of the salinity reduction on the relative permeability and capillary pressure curves, one of most relevant mechanisms for oil recovery by low salinity waterflooding at laboratory scale, are introduced as parametric changes in standard models. The model is based on some previous models [3][2]. Finally, the dynamics of the process is presented for some core flood study cases with different brine salinity.

References:


Click here to agree

Parallel 2-G / 90

Macroscale modeling of immiscible two-phase flows in highly permeable porous media

Sylvain PasquierNote; Michel Quintard1; Yohan Davit1

1 Institut de Mécanique des Fluides de Toulouse

Corresponding Author(s): yohan.davit@imft.fr

Multiphase flows in porous media play an important role in many natural and industrial processes, such as transport mechanisms in the vadose zone, CO2 sequestration in saline aquifers or oil recovery in petroleum applications. The traditional picture for such flows is one at low Reynolds number where the distribution and flow of the different phases is controlled by interfacial energies of fluid/fluid and fluid/solid interfaces, with a major influence of wettability and capillarity cite(Muskat1946,Whitaker1986). While this is accurate for creeping flows in relatively low permeability porous media, highly permeable porous structures –such as those found in trickle bed reactors, fuel bundles in nuclear cores or distillation columns used in chemical engineering applications– challenge the relevance of this representation. In those, the relative importance of interfacial energies may be reduced, with much larger inertial effects and exchanges of momentum between fluid phases.

Here, we discuss whether the continuum models used for flows in low permeability porous media, such as generalized Darcy’s laws, are adequate for highly permeable porous structures (high Re, Bo and We numbers). We first propose an alternative representation for mass and momentum transport of two-phase immiscible flow at the continuum-scale, which is based on a multiscale analysis starting from the flow problem at the pore-scale. Compared to the generalized Darcy’s law, our representation contains additional drag and cross terms that account for inertial effects and exchanges between fluid phases. We then go on to determine constitutive relationships for the effective parameters using experimental data on co- and counter-current flows from recent water/air experimental
data \cite{ClavierChikhiFichotEtAl2017,Wang_thesis}. Results show that the macroscale model allows us to capture important physical aspects of the flow that the generalized Darcy’s law fails to describe. We further find that the impact of the cross and inertial terms increases with the Reynolds numbers of the phases.

References:

@Article{Muskat1946,
Title = {The flow of homogeneous fluids through porous media},
Author = {M. Muskat},
Year = {1946}
}

@Article{Whitaker1986,
Title = {Flow in porous media II: The governing equations for immiscible, two-phase flow},
Author = {S. Whitaker},
Journal = {Transport in Porous Media},
Year = {1986},
}

@Article{ClavierChikhiFichotEtAl2017,
author = {R. Clavier and N. Chikhi and F. Fichot and M. Quintard},
title = {Modeling of Inertial Multi-Phase Flows through High Permeability Porous Media: Friction Closure Laws},
journal = {International Journal of Multiphase Flow},
year = {2017},
volume = "91",
pages = "243 - 261",
}

@PhdThesis{Wang_thesis,
Title = {Mass Transfer Coefficients and Effective Area of Packing},
Author = {C. Wang},
School = {University of Texas, Austin},
Year = {201},
Month = may
}

Acceptance of Terms and Conditions:

Click here to agree

**Poster 2 / 1098**

**Main controlling factors and development strategy of heterogeneity in platform carbonate reservoirs**

Yichang Yu\textsuperscript{None} ; Xinmin Song\textsuperscript{1} ; Rui Guo\textsuperscript{1} ; Hangyu Liu\textsuperscript{2} ; Fengfeng Li\textsuperscript{2}

\textsuperscript{1} Petrochina Research Institute of Petroleum Exploration and Development
\textsuperscript{2} Petrochina Research Institute of Petroleum Exploration and Development

**Corresponding Author(s):** yuyichang2013@163.com

The platform carbonate reservoirs in the Mishrif Formation of the HF Oilfield in Iraq are highly heterogeneous and can easily lead to water injection breakthrough along the high permeable thin layer to reduce the water injection sweep efficiency. Therefore, it is of great significance to clarify the main controlling factors of heterogeneity and formulate a reasonable development strategy. Based on conventional physical property, mercury injection capillary pressure test, casting thin sections, scanning electron microscopy, carbon and oxygen isotope analysis, combined with production dynamic and production-injection profile test, the heterogeneity characteristics caused by sedimentary and diageneisis and the corresponding development countermeasures are systematically
studied. The results show that: (1) The beaches in platform can be divided into shoal and inter-shoal, the shoal is mainly composed of bioclastic packstone and grainstone, while the inter-shoal is given priority to bioclastic wackestone. The types of bioclastic are mainly benthic foraminifera and rudist, including some echinoderm and bivalves. The shoal and inter-shoal is interactively distributed, and the single beach is a reverse cycle with a thickness of about 2-6m. (2) The bioclastic shoal is formed in the high position of strong hydrodynamic, the content of micrite is low, and the atmospheric freshwater dissolution is frequent during the diagenesis stage. It includes intergranular pore, intergranular dissolved pore, mould pore and intragranular pore, throat contains reduced-neck and silm throat with medium-high permeability. The inter-shoal is a lower area with deep water between shoals, with high micrite content and less freshwater dissolution at the diagenetic stage. In addition, dissolution product from the shoals results in calcium cement which blocking throat of the inter-shoal. It includes mould pore, intragranular pore and micropore, throat contains silm and cluster throat with low-permeability. (3) On the basis of sedimentation, diagenesis further enhances the heterogeneity of the reservoir, especially the top of the shoal turns into high permeability layer, accordingly inter-shoal becomes a region with low water seepage efficiency. During the development of waterflooding, the injected water quickly breakthrough along the top of the shoal, and the water content of the production well rises rapidly, meanwhile the production-injection profile test shows the monolayer breakthrough. (4) In the development strategy, the injection wells must avoid the high-permeability layer at the top of the shoal, and perforate in the lower part of the shoal and the whole inter-shoal, while all the production wells should be perforated in the whole beach. The reasonable development technology countermeasure effectively circumvents the high permeability layer may lead to rapid waterflooding and monolayer breakthrough, and have achieved good application effects.

References:

Click here to agree

Parallel 4-D / 256

Manual and Automated In Situ Contact Angle Measurements of scCO2 and Brine in Sandstone Cores Using Micro-CT Imaging - A Correlation to Pore Connectivity

Author(s): Laura Dalton

Co-author(s): Seth King ; Samantha Fuchs ; Dustin Crandall ; Angela Goodman ; Katherine Klique

1 U.S. Department of Energy National Energy Technology Laboratory
2 University of Texas at Austin
3 Sandia National Laboratory, Albuquerque, NM

Corresponding Author(s): laura.dalton@netl.doe.gov

Geologic Carbon Storage is one method available to mitigate excess carbon dioxide produced at point sources. X-Ray micro-computed tomography provides the resolution requirements necessary to image in situ contact angles (θ) at representative conditions; however, experimental data is limited and varies among materials and temperature settings used in literature (Andrew et al., 2014, Lv et al., 2017, Tudek et al., 2017). To further expand the practice of X-ray tomography, experiments were done on Mt. Simon and Nugget sandstone, adding more contact angles to the library of data obtained with this technique. The Mt. Simon core was subject to one imbibition cycle. The Nugget sandstone contained a preferential pathway spanning the length of the core and was further analyzed
to correlate the effect of connectivity to the resultant θ measurements. Two separate experiments were completed using the same Nugget core: (1) drainage and two imbibition cycles and (2) drainage and one imbibition cycle. In the first Nugget test, scCO₂ remobilized and became trapped in new pores along the flow path after the second imbibition cycle. Detailed analyses were completed for the Nugget sandstone: θ were measured and remeasured after the second imbibition cycle on scCO₂ ganglia that remained trapped between brine floods and θ within a pore were measured after each imbibition cycle to determine variation. For comparison with the Mt. Simon core, the sessile drop method was completed on additional Mt. Simon samples. The θ range was reviewed for both the Nugget and Mt. Simon where θ were measured manually in three different planes throughout each core and summed to an average value. The results were compared to determine any variation between sandstones. An automated algorithm designed to measure θ was developed to verify the sessile drop method results, to check the average θ values for both Nugget and Mt. Simon, and to measure more θ throughout the cores for more representative data. From manual measurements, Mt. Simon sandstone resulted in an average θ of 35° and a range from 5° to 120° while the Nugget sandstone resulted in an average θ of 56° and a range of 5° to 145°. The average contact angles for each classify both cores as weakly water-wet systems while the ranges suggest an intermediate-wet system within some pores. The Nugget average θ was 20° higher than the Mt. Simon sandstone and had a broader θ range by 25°. Different contact angles in two sandstone cores exposed to similar conditions indicate additional factors need to be considered.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 358

Manufacturing a micro-model with integrated fibre optic pressure sensors

Ioannis Zarikos¹ ; S. Majid Hassanizadeh¹ ; Lucas van Oosterhout¹ ; Wim van Oordt²

¹ Utrecht University
² Department of Chemical Engineering, Delft University of Technology, 2629 HZ Delft, The Netherlands

Corresponding Author(s): i.zarikos@uu.nl

ABSTRACT

Two-phase flow in porous media is a process encountered in various applications such as oil recovery, soil remediation, CO₂ sequestration and many other industrial systems. Multiphase flow in porous has been experimentally investigated with the use of micro-models, as well as natural porous media. Up to now, fluid pressure measurements during two-phase flow experiments in micro-models have been mainly performed in external lines or in inlet/outlet areas of the micro-model. For example, absolute or differential pressure between the inflow and outflow reservoirs of the micro-model has been measured with dedicated pressure sensors 1-3. However, external pressure measurements, despite being valuable, are not representative of the pressure distribution inside the micro-model pore space.
I order to achieve pore scale pressure measurements, we combined soft lithography and fibre optic pressure sensors. The PDMS micro-models was manufactured based on the procedure described by 4. The pressure sensors were miniature Fibre Optic Piezometers M260-SHEATHED (Smartec). These sensors had a diameter of 260mm and they were covered with a protective sleeve, resulting to an overall diameter of 320μm. Their measurement range is from ~40kPa up to 40kPa, with a resolution of 40Pa and accuracy of 0.6% of the full range, which makes them ideal for monitoring pressure at the pore scale. Moreover, the acquisition rate of 250Hz is sufficient for fast monitoring of pressure changes commonly encountered in dynamic two-phase flow experiments.

In this work, we describe the fabrication of a micro-model, made of PDMS, with integrated fibre optic piezometers. We demonstrate that these sensors provide pore-scale pressure measurements during two-phase flow. We show that the sensor shows an almost linear pressure distribution during steady-state single phase flow. The variation of pore pressure with time at each sensor location clearly show the effect of minor and major pore-filling events as well as breakthrough of the fluids when they reach the micromodel outlet.

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 928

Marangoni induced fracturing in two-dimensional frictional flows

Marcel Moura1; Guillaume Dumazer2; Fredrik Kvalheim Eriksen3; Knut Jørgen Måløy2; Eirik Grude Flekkøy3; Renaud Toussaint4

1 PoreLab, Department of Physics, University of Oslo
2 University of Oslo
3 Porous Media Laboratory
4 Institut de Physique du Globe de Strasbourg, University of Strasbourg/EOST, and PoreLab, Department of Physics, University of Oslo

Corresponding Author(s): marcel.moura@fys.uio.no

The competition between different driving forces (pressure gradients, gravity, internal friction, etc.) typically leads to various instabilities together with the development of a wide range of visually impacting patterns. The particular case of frictional flows, which consists in the displacement and structuring of a granular phase under viscous or capillary stress, can be considered as a deformable porous medium. Here particle-particle interactions are crucial, and major efforts have been put into characterizing the morphology and dynamics of developing fractures when the frictional fluid is deformed. Surface tension effects usually emerge as an opposing force to the fracture growth to minimize the growth of an interface. Typically, the condition for the development of a fracture is
that an external driving force (for example an imposed pressure difference) has to be higher than a certain threshold set by surface tension and/or internal friction. In this work we study the opposite scenario in which surface tension is forcing the fracture development. We employ a very simple table-top setup consisting of a two-dimensional suspension of particles located on the surface of a liquid. A gradient in surface tension is induced by use of a surfactant in the liquid. This perturbation is fracturing the homogeneous suspension and a flow is triggered along cracks. We have used high-speed and high-resolution techniques coupled to image analysis routines to study the emerging fracture patterns.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 271

Markov chain Monte Carlo Methods for Seismic Inversion

Georgia Stuart¹ ; Susan Minkoff² ; Felipe Pereira²

¹ The University of Texas at Dallas
² Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA

Corresponding Author(s): luisfelipe.pereira@utdallas.edu

Bayesian seismic inversion can be used to sample from the posterior distribution of the velocity field, thus allowing for uncertainty quantification. However, traditional Markov chain Monte Carlo (MéMC) can be extremely computationally expensive. In this presentation we compare recently proposed, computationally effective MéMC methods, such as a two-stage [1,2], a Hamiltonian procedure [3], and the DREAM [4], in examples where we consider both the modeling of the velocity field within geological layers as well as the identification of boundaries between such layers.

References:

Click here to agree

Parallel 4-A / 420

Mathematical model of kinetic mass transfer and transport of CO2 in shallow subsurface

Author(s): Jakub Solovský¹
Co-author(s): Radek Fučík² ; Tissa Illangasekare³ ; Michael Plampin⁴

¹ FNSPE, CTU in Prague
² Czech Technical University in Prague
3 Colorado School of Mines
4 U.S. Geological Survey

Corresponding Author(s): jakubsolovsky@gmail.com

In this work, we investigate CO2 exsolution, transport, trapping and dissolution in shallow subsurface under various conditions.
First, we introduce mathematical model describing the system. For the mass transfer of CO2 the rate limited model is used.
Numerical results obtained using the model are compared to the experimental data obtained from two sets of experiments: 1D column experiments and intermediate scale 2D experiments. In all the experiments water with dissolved CO2 was injected into the tank and the fate of dissolved and gaseous CO2 was observed.
The experiments were conducted under various conditions including different heterogeneity configurations, flow rates and dissolved CO2 concentration.
We investigated the effects of the different conditions in the experiment on the studied processes of exsolution, transport, trapping, and dissolution and addressed these dependencies in the mathematical model.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 361

Mathematical modeling of BTEX concentrations on the unsaturated zone using a simple finite differences model: evaluation of the mass distribution between phases

Author(s): JAVIER RODRIGO-ILARRI

Co-author(s): J. Jaime Gómez-Hernández ; Maria Elena Rodrigo-Clavero ; Anna Mafé Martí

1 UNIVERSITAT POLITECNICA VALENCIA
2 Universitat Politècnica de València
3 Universitat Politècnica de València

Corresponding Author(s): jrodrigoilarri@gmail.com

The impact of fuel spills on the unsaturated zone are one of the main environmental issues when licensing new fuel stations or industrial facilities where Underground Storage Tanks (UST) are used. The development and use of fate and transport models of organic pollutants (BTEX) on the vadose zone can therefore be used to understand the behavior of these pollutants under different scenarios.

This paper describes the results obtained when using a simple one-dimensional finite different vadose zone leaching model that describes the movement of organic contaminants within and between three different phases: (1) as a solute dissolved in water, (2) as a gas in the vapor phase, and (3) as an absorbed compound in the soil phase. The model uses a numerical approximation of the Millington Equation, a theoretical based model for gaseous diffusion in porous media. This equation has been widely used in the field of soil physics and hydrology to calculate the gaseous or vapor diffusion in porous media.

Initially, the equilibrium distribution of contaminant mass between liquid, gas and sorbed phases is calculated. Transport processes are then simulated. Liquid advective transport is calculated based on values defined by the user for infiltration and soil water content. The contaminant in the vapor phase migrates into or out of adjacent cells based on the calculated concentration gradients that exist between adjacent cells. After the mass is exchanged between the cells, the total mass in each cell
is recalculated and re-equilibrated between the different phases. At the end of the simulation, (1) an overall area-weighted groundwater impact for the entire modeled area and (2) the concentration profile of BTEX on the vadose zone are calculated.

The distribution of total mass of pollutants between the three phases is shown. A sensitivity analysis of the model parameters to a set of soil contamination scenarios caused by a set of BTEX spills from synthetic underground storage tanks is presented. Results demonstrate the applicability of simple numerical models for the environmental analysis of new industrial sites where soil contamination may be caused by organic pollutants.

References:
Ravi, V. and Johnson, J.A. VLEACH, A One-Dimensional Finite Difference Vadose Zone Leaching Model. Version 2.0. USEPA

Click here to agree

Parallel 10-B / 85

Mathematical modeling of microstructured membrane filters: A stochastic approach

Pejman Sanaei¹ ; Binan Gu² ; Lou Kondic² ; Linda Cummings²

¹ CIMS-NYU
² NJIT

Corresponding Author(s): ps160@nyu.edu

Membrane filters have been widely used in industrial applications to remove contaminants and undesired impurities from the solvent. During the filtration process the membrane internal void area becomes fouled with impurities and as a consequence the filter performance deteriorates, which indeed depends on filter internal structure, particles concentration and flow. The complexity of membrane internal morphology and stochasticity of particles flow make the filtration process and fouling mechanisms a mysterious phenomenon and hard to study. Therefore, mathematical modeling can play a key role in investigating filter fouling and discovering efficient filtration process. So far various mathematical models have been proposed to describe the complexity of membrane structure and stochasticity of particles flow individually but very few focus on both together. In this work, we present an idealized mathematical model, in which a membrane consists of a series of bifurcating pores, which decrease in size as the membrane is traversed and particles are removed from the feed by adsorption within pores (which shrinks them) and stochastic sieving (blocking by large particles). We discuss how filtration efficiency depends on the characteristics of the branching structure.

References:

Click here to agree

Parallel 4-D / 543

Maximising information on mudrock microstructure through high-resolution scanning electron microscopy

Shereef Bankole¹ ; Jim Buckman¹ ; Dorrik Stow²

¹ ²
Corresponding Author(s): shereef.bankole@pet.hw.ac.uk

Mudrocks are the dominant rocks in the Earth crust and are as well noted for their heterogeneity at several orders magnitude of scales. This implies a significant challenge in relating observations at varying scales to one another. A unique attribute that controls petrophysical properties of mudrocks is their microstructure which also controls fluid movement within them. Due to the fine-grained size of mudrocks, high-resolution measurement is required to reveal their microstructural characteristics. High-resolution scanning electron microscopy has advanced knowledge about microstructure of mudrocks but further development of fast and reliable methods to accurately determine the micron-submicron features of mudrocks is still on-going.

In this paper we present several information on mudrocks properties derived from scanning electron microscopy including grain size, grain-orientation, mineralogy and porosity, pore size distribution. The method involves multiple large-area, high-resolution scanning electron microscopy through automated acquisition and stitching of backscattered images (BSE) from polished thin-sections in combination with machine learning segmentation and energy dispersive X-ray analysis (EDX). Preliminary results obtained from the methodology was applied to seven mudrocks from deep-water identified as hemipelagites from the New Zealand Continental Slope (IODP Expedition 317) and Iberian Peninsula (IODP Expedition 339).

Grain size analysis shows that all the samples are within silt-mud class size. Orientation analysis indicates that randomly representative areas within each sample are heterogeneous; displaying a combination of preferred orientation direction and random orientation. The samples were differentiated into clay dominant and calcite dominant based on EDX. Porosity on representative areas for individual samples are heterogeneous reflecting areas that are tightly porous, partially porous and highly porous area. Interestingly, calcite dominated samples showed tighter porosity compared to clay dominated samples. However, there is no significant difference among representative areas per sample in terms of pore size distribution.

Automated image analysis of large area, high-resolution montages presented herein, is fundamental to revealing heterogeneity and deriving plethora of information on mudrock microstructure. The process minimises human subjectivity and bias but the limitations to the workflow are the time involved for individual runs and large amount of computer memory required. In addition, cracks in the sediment samples resulting from drying, preparation of polished thin-section as well as stress relaxation during coring, restrict the area available for high-resolution large-area imaging to that between the cracks. This method is very significant for improved understanding of subsurface mudrocks and their capacity for fluid movement and storage.

References:

Acceptance of Terms and Conditions:

Click here to agree

Measuring and Modelling Supercritical Gas Adsorption in Clay Minerals and Shales

Author(s): Ronny Pini¹

Co-author(s): Lisa Joss¹; Junyoung Hwang¹; Humera Ansari¹

¹ Imperial College London

Corresponding Author(s): r.pini@imperial.ac.uk

Clay minerals are ubiquitous in the subsurface: they are found in CO2 sequestration targets (e.g., sandstones) and in the seals above them, and are major constituents of unconventional shale plays considered for natural gas recovery. A significant fraction of the porosity in clay-rich systems is
occupied by micro- and meso-pores that provide a large surface area for physical and chemical interactions with the surrounding fluids. Of particular interest to this study is the adsorption behaviour of CO2 and CH4 that leads to the trapping of these gases in the porous structure at liquid-like densities. From a practical perspective, gas adsorption can lead to (i) an increase of storage capacity in reservoirs having larger clay contents, (ii) an advance in storage safety by limiting gas diffusion through cap rock seals, and (iii) an enhancement of gas production from tight shale formations through an adsorption/desorption (CO2/CH4) process.

Supercritical gas adsorption studies on clay and shale samples that address these aspects are found in the literature, but the picture is still far from being complete. The main reason for this is the intrinsic difficulty in performing these experiments at subsurface conditions (high-pressure and temperature), and in their description, because the interactions between the gases and the rock’s constituents (clays, carbonate minerals and organic matter) are quite complex. The lack of a systematic evaluation on the effects of temperature, pore structure and pore chemistry on gas adsorption over the relevant pressure range precludes the development and validation of theoretical models for gas adsorption in rocks that have a sufficient degree of predictive ability. The latter is a necessity if laboratory observations that are inevitably limited in their probed rock volume are to be used to make useful estimates of process-relevant parameters, such as Gas-In-Place and storage capacity. We report results from a systematic experimental investigation on the adsorption properties of CO2 and CH4 over a wide range of conditions (0-25 MPa and 40-80°C). The systems considered include pure clay minerals (e.g., Na-montmorillonite), shale samples from various (potential) plays (Eagle Ford, Utica and Bowland Shale), as well as reference materials with well-defined surface chemistry and pore structure (micro- and meso-porous zeolites, carbons and silica). Data are interpreted using appropriate quantitative measures, such as the excess adsorption and Henry constants. The measured adsorption isotherms are described using a Lattice Density Functional Theory (LDFT) model that uses as input parameter the pore structure of the material (measured from conventional cryogenic adsorption experiments). As such, the modelling approach is more rigorous, has predictive capability and represents a significant departure from conventional empirical approaches that use Langmuir- or BET-type of models.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-C / 177

Mechanical Degradation of Polymer Solution in Micro Pore Throat

Lijuan Zhang1; Xiangan Yue2; Shengxu Zhao3

1 China University of Petroleum, Beijing, China
2 China University of Petroleum

Corresponding Author(s): zhangljbj2001@sina.com

The oil displacement effect of polymer flooding is mainly governed by the rheological property of polymer in the deep reservoir, while the mechanical degradation is one of the key factors affecting its rheological properties. Polymer molecular chains can be mechanically degraded in shear flow and extensional flow, which both involves in the flow through a porous medium. Mechanical degradation includes shear degradation and stretch degradation. The questions are which one dominates, the shear or the stretch, how much it degrades, and how to simulate.

Maerker [2] conducted degradation of partially hydrolyzed polyacrylamide (HPAM) through consolidated sandstone plugs and reported that the degradation of HPAM through porous media was caused by large viscoelastic normal stress in elongational flow field and larger flow rate, longer flow distance and lower permeability induced more severe degradation. Dupas et al. [3] carried out HPAM degradation experiments through an API (American Petroleum Institute) capillary system, indicated that after polymer was degraded at velocity 8m/s, shear viscosity drops by 10%, while extension viscosity decreases up to 60%.

The objective of this work is to develop a device to simulate the mechanical degradation of polymer in micro pore throat, identify the shear effect and elongational effect, examine the viscosity loss of
polymer solution through different pore throat model and present the relationship between viscosity loss and extensional rate. Mechanical degradation is induced by forcing fresh polymer solution through a device which consists of a series of pore throat models with 4 kinds of throat length (15mm, 35mm, 70mm, 100mm) and 3 kinds of diameter (100μm, 300μm, 500μm). Viscosity measurement of native and degraded polymer solution is made with Haake RS6000 rheometer at 25°C. The throat flow rate varies from 6.37 m/d to 3821.66 m/d. Polymer is HPAM with intrinsic viscosity 2510 dL/g. The concentration of polymer is 250mg/L, prepared in brine with salinity 32868 mg/L. Viscosity loss caused by extensional degradation can be obtained by calculating the viscosity loss of polymer solution degraded through pore throat model with throat length 0 mm. Accordingly, viscosity loss caused by the shear degradation through pore throat model with different throat length is calculated. The results show that there is no obvious correlation between viscosity loss of HPAM in the pore throat model and throat length. More than 95% viscosity loss is caused by stretching degradation in pore throat, which is the main mechanism of mechanical degradation. The relationship between viscosity loss in pore throat and extensional rate (ε) has two characteristic values (ε0 and εL). ε0 is the critical extensional rate, εL is the ultimate extensional rate. When ε < ε0, the viscosity of polymer solution decreases slowly; when ε0 < ε < εL, the viscosity drops sharply; when ε > εL, viscosity loss keeps unchanged. ε0 and εL can be used as index parameters to evaluate anti-mechanical degradation ability of oil displacement polymer.

References:

Click here to agree

Parallel 1-C / 171

Mechanisms Limiting Plugging of Near-Borehole Cracks with Bentonite

Andrew Bunger1; Rachel Asit Upadhyay1; Carolyn Wehner1; Mohammad Nurul Islam2

1 University of Pittsburgh
2 National Energy Technology Laboratory

Corresponding Author(s): bunger@pitt.edu

The effectiveness of bentonite clay as a wellbore plugging material often depends upon its penetration into near-borehole cracks associated with the drilling process. Here we present research aimed at understanding and maximizing the ability of clay materials to plug near-borehole cracks. A device was constructed such that the borehole is represented by a cylindrical chamber, and a near-borehole crack is represented by a slot adjacent to the center chamber. The experiments consist of placing bentonite clay pellets into the center chamber and filling the entire cavity with distilled water or brine so that the pellets hydrate and swell, thereby intruding into the slot. Results indicate that the bentonite clay pellets do not fully plug the slot. We propose a model where the intrusion length into the slot is limited by: 1) the free swelling potential intrinsic to the system comprised of the bentonite pellets and the hydrating fluid, and 2) the resisting shear force along the walls of the slot. This model accounts for the fact that narrow slots have a smaller volume for the clay to fill than wider slots, but wider slots present less resistive force to clay intrusion. These two limiting mechanisms work against each other, leading to a non-monotonic relationship between slot width and intrusion length. Specifically, the results show a linear increase of the intrusion length with the slot width for narrow slots where the limit is the shear strength resisting intrusion and scaling in proportion to the slot width over which the driving swelling pressure is applied. For wide slots the intrusion length is controlled by available swelling volume and scales inversely with the volume of the slot,
and hence also inversely with the slot width. The experiments also show that increasing the salinity of the solution leads to a dramatic decrease in the clay expansion, evidenced here by the substantially smaller intrusion length when the pore fluid contains 10 g/L NaCl. We conclude that there exists a range of length to width ratios of near wellbore cracks that will be effectively plugged, and where a suitable plugging criterion is determined by a competition between availability of volume and shear resistance to clay intrusion.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 1067

Melting temperatures and solubilities of congruently melting salt hydrates confined in nanoporous materials

Michael Steiger*; Tobias Grünzel*

Corresponding Author(s): steiger@chemie.uni-hamburg.de

The Gibbs energy of nanocrystals increases with decreasing crystal size due to an increasing surface to volume ratio (A/V) resulting in a solubility increase and a melting temperature decrease of small crystals. In the case of pure phases, the melting temperature decrease may be approximately represented by the Gibbs–Thomson (GT) equation. However, the melt of a salt hydrate is not a pure phase but rather a concentrated electrolyte solution. Hence, the GT equation does not apply and a different approach based on the solubility increase of small crystals is used here. The additional energy of a small crystal is accounted for by the surface energy yielding an expression for the solubility increase of nanocrystals. For the thermodynamic solubility product of small crystals we obtain:

\[
\ln K = \ln K_0 + (c_1 V_m/RT) (dA/dV) \tag{1}
\]

where \( K \) and \( K_0 \) are the thermodynamic solubility products of the small and an infinitely large crystal, respectively, \( c_1 \) is the surface free energy of the crystal–liquid interface, \( V_m \) is the molar volume of the solid, \( R \) is the gas constant and \( T \) is the absolute temperature. The surface to volume ratio is inversely proportional to the crystal size. For a spherical crystal of radius \( r \), \( dA/dV = 2/r \). The solubility curve of a hydrated salt, i.e. the relation between composition of the saturated solution and temperature, is a continuous function with a maximum if temperature is the ordinate and composition the abscissa. The maximum of the curve is the melting temperature of the hydrated solid and the composition of the saturated solution (the solubility at the melting temperature) equals the composition of the solid. Therefore, as shown in Fig.1, the melting temperature decrease \( T_m \) of a small crystal corresponds to a solubility increase \( \Delta s \). Thus, the solubility increase of small crystals can be determined indirectly by measurement of the melting temperature. In the present study, we have determined the melting temperatures of nanocrystals of \( \text{M(NO}_3\text{)}_2\cdot6\text{H}_2\text{O} (M=\text{Mg,Zn}) \), confined in mesoporous materials with narrow pore size distributions and different pore diameters (Vycor glass, mesoporous silica). Using a molality based Pitzer model for the calculation of water activity and activity coefficients, the thermodynamic solubility products of the nanocrystals were calculated. Using Eq. (1) and treating \( c_1 \) as an adjustable parameter, the data were used to determine values of the surface free energy of the crystal–liquid interface.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-B / 217

Membrane morphology and topology: Fouling control in filtration systems
Author(s): Bowen Ling

Co-author(s): Ilenia Battiato

1 Stanford University

Corresponding Author(s): bowenl@stanford.edu

Reverse Osmosis Membrane (ROM) filtration systems are widely utilized in waste-water recovery, seawater desalination, landfill water treatment, etc. During filtration, the system performance is dramatically affected by membrane fouling which causes a significant decrease in permeate flux as well as an increase in the energy input required to operate the system. Design and optimization of ROM filtration systems aim at reducing membrane fouling by studying the coupling between membrane structure, local flow field and foulant adsorption patterns. Yet, current studies focus exclusively on oversimplified steady-state models that ignore any dynamic coupling between fluid flow and transport through the membrane. In this work, we develop a customized solver (SUMs) under OpenFOAM to solve the transient equations. The simulation results not only predict macroscopic quantities (e.g. permeate flux, pressure drop, etc.) but also show an excellent agreement with the fouling patterns observed in experiments. It is observed that foulant deposition is strongly controlled by the local shear stress on the membrane, and channel morphology or membrane topology can be modified to control the shear stress distribution and reduce fouling. We demonstrate how channel morphology and membrane topology can be jointly optimized in order to increase the efficiency of the system. Finally, we identify optimal regimes for morphological and topological modifications in different operation conditions.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-F / 16

Mesoscopic simulation and characterization of the morphological evolution in phase separating fluid mixtures

Manuel Hopp-Hirschler1; Christian Zander1; Ulrich Nieken

1 University of Stuttgart

Corresponding Author(s): manuel.hopp@icvt.uni-stuttgart.de

In several applications, morphology evolves over time, e.g. in the formation of pores in porous polymer membranes or in the formation of porous particles during spray polymerization of suspensions in a drying chamber. For example, during the preparation of porous polymer membranes by phase inversion process, a homogeneous polymer solution phase separates at contact with a coagulation bath due to a miscibility gap. A polymer rich and a polymer lean phase, representing membrane matrix and pores, are formed. The shape of the morphology can be very different depending on the material properties and process conditions.

A direct quantitative comparison of the morphology of porous polymer membranes in experiments and numerical simulations is not possible because of the stochastic nature of the origin of phase separation. A reasonable way to compare different morphology is to compare the characteristics of the morphology. In the context of phase separating fluids, Minkowski functions, Betti numbers, interfacial shape distributions and Doi-Ohta mapping [2] were used to characterize morphology. The latter approach was originally introduced in rheology by Doi & Ohta [3] to describe morphological dependent viscosity of polymer blends. We use Doi-Ohta mapping to characterize the morphology during phase separation because an advantage of the Doi-Ohta approach is that it offers a thermodynamic-consistent evolution equation of the characteristics of the morphology by reducing the Cahn-Hilliard level to a macroscopic level.

The aim is to extend the Cahn-Hilliard-SPH model proposed earlier by some of the authors [4] to account for thermal fluctuations in the concentration by adapting the form of thermal noise suggested in [5]. The result is a thermodynamically consistent model for diffusion controlled phase separating
fluid mixtures for engineers, which can be used to investigate the evolution of anisotropic morphology from initially homogeneous fluid mixtures. We simulate different morphology, characterize the anisotropic nature by Doi-Ohta mapping and conclude that the characteristics of the anisotropy is well captured in the Doi-Ohta approach.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 3-A / 347

Methane Migration in Water Saturated Formations — Applications to CO2 Sequestration and Groundwater Contamination from Leaky Natural Gas Wells

Author(s): Joachim Moortgat¹
Co-author(s): David E Graham ²; David R Cole ¹; Franklin W Schwartz ²; Mohamad Reza Soltanian ¹; Mohammad Amin Amooie ¹; Susan M Pfliffter ²; Thomas H Darrah ¹; Tommy J Phelps ²

¹ The Ohio State University
² Oak Ridge National Laboratory
³ University of Tennessee, Knoxville

Corresponding Author(s): moortgat.1@osu.edu

Target formations for large-scale CO2 sequestration are often saturated with brines that contain dissolved methane and other light hydrocarbons. When CO2 is injected in such deep formation, non-trivial phase behavior may result in methane exsolving from the brine and forming a free gas phase. Because methane has a lower viscosity than the (generally supercritical) CO2, this methane-rich gas is swept up ahead of the CO2 front. On the one hand, such a ‘bank’ of methane may provide an early tracer warning of the approaching CO2 plume, e.g. in observation wells. On the other hand, the emergence of gaseous methane poses risks of releasing a potent (groundhouse) gas contaminant in overlying groundwater and potentially the atmosphere if the formation integrity is compromised by (open) fractures, faults, or leaky wells.

The transport of methane in water-saturated formations is also important in the context of natural-gas production from deep reservoirs. If a producing well is compromised, e.g., at shallower depths, leaking stray natural-gas may contaminate groundwater resources. Whether this contamination occurs in a small radius around the well (due to buoyancy) or travels significant distances laterally before contaminating groundwater wells depends strongly on the formation heterogeneity, notably fractures.

The modeling of these important processes is complicated by 1) strong heterogeneity in fluvial target formations for CO2 storage and fractured groundwater aquifers, and 2) the complicated phase behavior of mixtures of water and hydrocarbons. The latter can be modeled accurately by the cubic-plus-association (CPA) equation of state (EOS), which takes into account the polar nature of water molecules, its self-association, and the polar-induced cross-association between water, CO2, and methane molecules (as well as compressibility of the aqueous phase). While accurate, the CPA EOS
is highly non-linear and computationally expensive. In this work, we develop new efficient algorithms to adopt the CPA EOS for large-scale simulations. Flow and transport are modeled by the mixed hybrid and discontinuous Galerkin methods, respectively, and discrete fractures are incorporated through a cross-flow equilibrium approach.

Simulation results are presented for 1) the Cranfield large-volume CO2 storage pilot project, and 2) for lateral migration of stray methane leaking from a compromised natural-gas well into shallow fractured groundwater aquifers for conditions representative of those overlying the Barnett formation in Texas.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-G / 24

Methods for extracting Lagrangian coherent structures from unsteady velocity data

Sanjeeva Balasuriya¹

¹ University of Adelaide

Corresponding Author(s): sanjeeva.balasuriya@adelaide.edu.au

The fact that examining Eulerian entities in unsteady velocity fields gives misleading information on Lagrangian coherence is now well-established. In this talk, I will review a range of techniques which have been proposed to extract coherent structures from given velocity data. These include the commonly used finite-time Lyapunov exponents, as well as methods such as curves/surfaces to which there is maximal attraction, transfer (Perron-Frobenius) operator methods for identifying sets which are coherent to transport, clustering methods which group similarly behaving particles, Lagrangian-averaged vorticity for identifying vortices in a frame-independent fashion, and sets which are most susceptible to random perturbations. Each seeks different characteristics, and thus the appropriate method for a given problem needs to be chosen carefully. These methods—not currently well-known in the porous media community—may offer new approaches for extracting coherence in porous flows.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 682

Micro-PIV Measurements of Pore-Scale Flow of Water and Supercritical CO2 in 2D Circular Porous Micromodels at Reservoir Conditions

Yaofa Li¹; Farzan Kazemifar²; Gianluca Blois³; Kenneth Christensen¹; Yu Chen¹; Amir Kohanpur³; Albert Valocchi⁴

¹ University of Notre Dame
² California State University Sacramento
³ University of Illinois at Urbana-Champaign
⁴ Univ Illinois
Multiphase flow in porous media is relevant to a range of applications in the energy and environmental sectors. Recently, the interest has been renewed by geological storage of CO2 within saline aquifers. The coupled flow dynamics of CO2 and brine in geologic media must be better understood, particularly at the pore scale, because pore-scale phenomena, such as Haines jumps and shear-induced flows, represent a critical component of accurate large-scale modeling and predictions. Recent evidence also shows that wetting properties of the porous matrix significantly affect the multiphase flow and transport in porous media, and therefore challenges microscopic and macroscopic descriptions. To this end, the pore-scale flow interactions of water and liquid/supercritical CO2 are presently being quantified in 2D circular porous micromodels at reservoir-relevant conditions (i.e., 80 bar, 21°C), in an attempt to accurately mimics the process of CO2 injection into saline aquifers. The circular micromodels used in these experiments were fabricated from silicon, with the porous matrix formed with arrays of 2D poly-disperse cylinders. Circular micromodels (i.e., radial displacement) are superior to rectangle ones (i.e., linear displacement), in the context that the former ones reduce boundary effects that are inherent in linear displacement. Fluorescent microscopy and the micro-PIV method are employed by seeding the water phase with fluorescent particles and tagging the CO2 phase with a fluorescent dye. Doing so allows for simultaneous measurement of the spatially-resolved instantaneous water velocity field and quantification of the instantaneous spatial configuration of both phases [1]. High-speed cameras and a fast differential pressure transducer are used in order to temporally resolve the pore-scale flow. These spatially and temporally-resolved data are invaluable and imperative to understand the dynamics of certain pore-scale phenomena, such as Haines jumps, which occur with a time scale of no more than a few milliseconds [2]. Finally, measurements are performed under a variety of wettability conditions, in order to quantify the impact of wettability on the physics and to evaluate the role of capillary effects.

References:


Acceptance of Terms and Conditions:

Click here to agree
relative permeability from Darcy’s law. A numerical simulation model is developed to verify the assumptions of the streamtube dimension reduction technique. A variation of the reactor ratio is presented as an analytical metric to quickly determine the validity of the streamtube approximation in core and column-scale experiments. This study introduces an entirely new method for sub-core permeability and relative permeability quantification, and provides a foundation for future work on experimental measurements of differences in transport behavior across scales.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 307

Micro-scale effect of CO2 diffusion on two-phase flow in dual-porosity of tight oil reservoirs

Shouya Wu¹ ; Zhaomin Li¹ ; Chao Zhang¹ ; Guangzhong Lv² ; Songyan Li¹ ; Chenyu Qiao¹ ; Meijia Wang¹

¹ School of Petroleum Engineering, China University of Petroleum (East China)
² Research Institute of Petroleum Exploration and Development, Shengli Oilfield Company, SINOPEC

Corresponding Author(s): wushouya@upc.edu.cn

Carbon dioxide (CO2) diffusion in dual-porosity plays a great important role for effective flow in tight oil reservoir. The CO2 diffusion coefficient in matrix is different with the coefficient in fracture because of micro-scale effect. Matrix diffusion coefficient and fracture diffusion coefficient was introduced and respectively used into matrix flow model and fracture flow model. Using pressure drop method, matrix diffusion coefficient in tight porous media was determined by soaking the oil-saturated core in CO2 filled container with constant temperature. This paper developed a two-phase flow model in dual-porosity media coupling with two CO2 diffusion equations, and solved by Finite Difference Method (FDM). To reveal the scale effect, the results of two different numerical models were compared: (1) matrix diffusion coefficient equals to fracture diffusion coefficient; (2) matrix diffusion coefficient differ to fracture diffusion coefficient. Finally, this study verified the micro-scale effect on fluid flow in tight formations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 406

Microbial life in unsaturated porous media: a microfluidic approach

Author(s): Dorothee Luise Kurz¹

Co-author(s): Eleonora Secchi ¹ ; Vicente Fernandez ¹ ; Roman Stocker ¹ ; Joaquin Jimenez-Martinez ²

¹ ETH Zürich
² EAWAG-ETHZ

Corresponding Author(s): dkurz@ethz.ch

Soil is a complex environment in which the presence of several phases creates numerous interfaces (solid-liquid, liquid-gas and solid-gas). Understanding the local hydrodynamics in soil pores and the
biogeochemical processes such as nutrient cycling has been of growing importance in the field of bioremediation and ecology. Besides the coexistence of two immiscible phases (air and water) in the pore space, microorganisms, especially bacteria, are often found in large numbers in natural soil environments. The complex spatial distribution of air and water results in the development of a mosaic of regions of very low water velocity, including areas where water or air is trapped and of preferential channels of high velocity. This landscape of conditions enables microorganisms to live in the free-swimming phase and to form surface attached communities known as biofilms.

At the same time, the biofilms’ structure influences pore geometries resulting in altered hydrodynamics, affecting biofilm development and therefore mass transport. To study influences of soil conditions on biofilms and vice versa, we have studied two soil-born microorganisms, Pseudomonas and Bacillus, at the pore scale using microfluidic devices. We have explored the biofilm forming behavior under different physical conditions such as varied water saturation and flowrate. Carefully designed channel geometries coupled with automated video microscopy allowed us a zoomed-in view on specific interactions while controlling the water saturation by varying the gas flow into the channel. The simplified geometries of the devices resulted in a varied biofilm growth caused by the presence of an immiscible phase.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-B / 600

Microbially Induced Desaturation and Precipitation (MIDP) via Denitrification during Centrifugal Loading

Caitlyn Hall\textsuperscript{none} ; Leon van Paassen\textsuperscript{1} ; Bruce Rittmann\textsuperscript{1} ; Edward Kavazanjian\textsuperscript{1}

\textsuperscript{1} Arizona State University

Corresponding Author(s): cahall13@asu.edu

Microbially induced desaturation and precipitation (MIDP) via denitrification has the potential to mitigate earthquake-induced liquefaction by two mechanisms: biogenic gas production to desaturate and dampen pore pressure changes in soil and calcium carbonate precipitation to mechanically strengthen soil. Lab-scale tests have demonstrated that both desaturation and precipitation are effective mitigation mechanisms. However, small-scale laboratory column tests at ambient pressure lead to gas pockets and lenses, causing upheaval due to low overburden pressures. Therefore, biogenic gas formation, distribution, and retention need to be evaluated with more realistic over-burden pressures to understand the effectiveness of this treatment mechanism. Centrifuge tests of soil de-saturated by MICP treatment are currently being performed to simulate field pressures and stresses. In addition, a numerical model was developed to evaluate the scaling effects on biogenic gas generation between the centrifuge model and prototype scale. The centrifuge tests are conducted within a laminar box on the 1-m radius centrifuge at the University of California, Davis NHERI/CGM centrifuge facility. Desaturation is induced in the laminar box prior to acceleration in the centrifuge by augmenting saturated soil with an enriched culture of denitrifying microorganisms. The models are accelerated to 80 g in stages and measurements of soil moisture content are made over time to see the combined influence of steady-state pore pressure and overburden pressure on the degree of saturation. Upon reaching the final centrifuge acceleration, the models are subjected to strong shaking until either liquefaction is triggered or the capacity of the centrifuge is reached. Test results provide evidence of the capacity for MIDP to mitigate the potential for earthquake-induced soil liquefaction by desaturation. Comparison of modeling results to test data suggest that the numerical model does not consider certain pore-scale influences and the effects of mixing from liquid-gas transfer and transport observed in the centrifuge tests. Thus, future work will add these features to the model.

References:
Acceptance of Terms and Conditions:
Parallel 2-C / 747

Microbiological underground methanation: principle, bio-chemical and hydrodynamic models, and self-organization phenomena

Mikhail Panfilov¹ ; NOURA EDDAOUI²

¹ Université de Lorraine

Corresponding Author(s): eddaouinoura@gmail.com

A new technology is proposed, which consists of injecting H₂, CO₂ and bacteria into aquifers or depleted gas/oil reservoirs in order to convert them into methane. The conversion occurs by means of bacteria, which use hydrogen and carbon dioxide for their respiratory metabolism. The product of this bio-chemical activity is methane. Thus, we deal with the creation of the artificial reservoirs of natural gas. This also resolves two other fundamental environmental and energy problems: (i) reducing CO₂ emissions into the atmosphere by converting CO₂ to methane; and store excessively generated electricity from wind and sun in the form of hydrogen (this excess electricity can be converted to hydrogen).

The coupled bio-chemical and hydrodynamic model of the system is developed. The particular attention was payed to the adequate description of the bacterial kinetics and bio-chemical reactions. The mathematical analysis of this model revealed the existence of the phenomena of self-organization caused by the Hopf-Andronov bifurcation. This leads to the appearance of space oscillatory waves of concentration having multi-scale structure. Depending on the structure of these oscillations, they may be favourable or not for the efficiency of the methane production. Thus, the criteria of the efficiency of the underground methanation are strictly related to the mathematical criteria of the existence of self-organization regimes. Such exact criteria of the appearance of the auto-waves have been obtained. They depend on the injection rate, on the composition of the injected gas, and on the bacterial kinetics. Due to the analytical and numerical simulations, we have obtained the estimations for essential parameters of this technique, as the optimal composition of the injected gas, the characteristic time of conversion, and the evolution of the composition of the resulting gas in time.

References:

1. Panfilov M. Physicochemical fluid dynamics of porous media (with applications to geosciences and oil engineering). Wiley & Sun, 2018 (in edition)


Acceptance of Terms and Conditions:

Poster 3 / 643

Microfluidic Evaluation of the Effects of Wettability on Two-Fluid Flow in Porous Media

Kelsey Bruning¹ ; Sarah Kalkowski¹ ; Cass T. Miller¹

¹ University of North Carolina - Chapel Hill

Corresponding Author(s): kbruning@live.unc.edu
Subsurface systems are well known to have variations in wettability. Evolving models to describe such systems must be evaluated and validated, and highly resolved experimental observations can play a central role in this endeavor. Quantities such as interfacial areas and curvatures are examples of quantities that are not often measured in high resolution as a function of wettability. Displacement experiments for two-fluid-flow through microfluidic cells with a controlled wettability are reported and saturations, interfacial areas, and curvatures are examined in high resolution and time scales. The relaxation to an equilibrium state is quantified and shown to be long compared to the typical duration of such experiments.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-F / 892

**Micromodel study of low salinity water flood and wettability alteration**

Author(s): YUJING DU

Co-author(s): Ke Xu; Matthew Balhoff

1 University of Texas at Austin

Corresponding Author(s): yujingdu@utexas.edu

Low salinity water flooding is an effective and cost-efficient improved oil recovery method. Wettability alteration is believed by many to be the primary reason for the observations of increased recovery. However, the causes of the wettability alterations and approaches for optimization are not fully understood. We conduct experiments in micromodels by injecting brine at different salinities in these oil-saturated micromodels and observe distinct changes in the contact angle and wettability. Meanwhile, we observe water droplets form and grow with time inside the oil phase when low salinity water was injected. Additionally, significant improvements in oil recovery is observed when high-salinity brine is followed by low-salinity brine, but the response is delayed by hours or even days.

We fabricated glass, water-wet micromodels (homogeneous porous medium and single channel with dead-end) using the method we developed in Ke et al. [2017]. The micromodels are unique in that pores and throats are of different depths, thereby having three-dimensional features that allow oil snap-off behaviors. We conduct dead-end micromodel experiments and homogeneous micromodel experiments to see the oil recovery. For the dead-end micromodel experiments, visualization was conducted under microscope. Micromodels were initially saturated with crude oil (120 cp heavy Middle Eastern oil) and then flooded at very low rate by low salinity water (500 ppm) or high salinity (34000 ppm) water. For the homogeneous micromodel experiments, visualization was conducted under a digital camera. Micromodels were initially saturated with crude oil and then displaced by a high salinity sea water (34000 ppm) at 2 ft/day into micromodels until no additional oil was recovered. Then, low salinity (0-5000 ppm) water was injected at 2 ft/day into the micromodel for at least 2 days.

The dead-end experiments show that the micromodel was initial oil wet and gradually altered to more water wet after the low salinity water injection. We also observed water droplets forming and growing in the crude oil phase and oil swelling. This swelling appears to provide an additional mechanism for recovery.

From the homogeneous micromodel experiments, we observed up to 30% incremental oil recovery using the low-salinity brine after the high-salinity brine. Importantly, a time delay of hours even days was required. For zero-salinity (DI water) case we observed a more than 10 hours of flooding was required before production re-started, and more than 20 hours of delay for 5000 ppm brine.
Our conclusion is that the wettability alteration is a time dependent process caused by the redistribution of negative charged polar compounds within the crude oil. When low salinity water is injected, the polar compounds migrate from the surface to the inside of the oil and form micelles. The lack of polar compounds on oil surface leads to wettability alteration, and the water molecules accumulate around these micelles to form water droplets. The growing of water droplets leads to oil swelling which also contribute to the incremental oil recovery. The wettability alteration and the oil swelling are both consequences of the redistribution of the polar compounds, and both contribute to the additional oil recovery by both wettability alteration and oil swelling.

**References:**

Ke, et al. A 2.5-D glass micromodel for investigation of multi-phase flow in porous media, Lab Chip, 2017, 17, 640-646

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 2-E / 949**

**Microscale Modeling of the Effect of Silica nanoparticles and Surfactants on HeavyOil Displacements**

Parisa Bazazi¹ ; Amir Sanati Nezhad² ; S. Hossein Hejazi¹

¹ Subsurface Fluidics and Porous Media Laboratory; Department of Chemical and Petroleum Engineering; University of Calgary

² BioMEMS and Bioinspired Microfluidic Laboratory; Department of Mechanical and Manufacturing Engineering; University of Calgary

**Corresponding Author(s):** shhejazi@ucalgary.ca

Chemicals in the form of nanoparticles or surfactants provide opportunities to improve oil displacement from rocks. They increase the rate of hydrocarbon recovery by breaking down the oil trapped in by-passed zones and separating the residual oil from rock surfaces in the form of tiny droplets suspended in the water phase. In this study, a series of heavy oil displacement experiments are conducted by flowing a series of aqueous solutions through an oil-wet and transparent network of microfluidic devices. Micromodels are fabricated by soft lithography techniques on a silicon wafer and replicated with Polydimethylsiloxane (PDMS) polymer. The effect of silica nanoparticles and three different types of surfactants (SDS, Tween 20, and Silwet) on the displacement of heavy oil, removal of oil films, and mobilization of trapped oil droplets are investigated. Furthermore, the patterns of residual oil and final oil recovery factors are explored. Also, the synergism effect between nanoparticles and different types of surfactants are reported. 3D Confocal microscopy coupled with fast speed fluorescent imaging of the displacement process reveals the effect of each chemical additive on oil mobilization. Silica particles show the tendency to reduce or remove the remaining oil film thickness while the surfactants break up the oil phase in the by-passed channels into tiny clusters that can be transported by the displacing fluid. The results demonstrate that the addition of the silica nanoparticles increases the rate of oil recovery up to 60% resulted from the wettability alteration and oil film removal. Moreover, the recovery factors increase upon adding the silica nanoparticles to a constant concentration of Tween 20 and SDS. The silicon-based surfactants improve the oil recovery up to 80% where the recovery improvement by the addition of nanoparticles is negligible.

The developed microfluidic-based model is a powerful mimetic prototype of real porous media which can clarify the mechanisms underlying the process of chemical-based flooding for oil recovery. Considering the time-consuming and expensive nature of core-flood experiments, the proposed microfluidic approach provides an attractive alternative for rapid and low-cost enhanced oil recovery (EOR) screening studies.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree
Microstructural Modeling and Simulation of Heat Transfer in Wood Fiber based Insulating Materials

Author(s): Sarah Staub1
Co-author(s): Heiko Andrä1

1 Fraunhofer ITWM

Corresponding Author(s): sarah.staub@itwm.fraunhofer.de

Wood fiber based materials are of high interest in building insulation. Their application is desirable due to the sustainability of renewable resources. Furthermore, wood fiber based materials outmatch petrochemical based materials with respect to health aspects during process and application.

The insulation properties of such fiber based materials are often characterized experimentally, which has certain disadvantages. For instance, the experimental characterization requires a high effort to characterize only few produced material variants. The connection between the properties of the fibrous microstructure and the effective thermal conductivity is hardly enlightened.

To overcome these disadvantages in the current presentation a microstructural modeling and simulation approach for the determination of the effective heat transfer is presented. The development of imaging procedures and powerful computer simulations allow the characterization of structure property relationships even for highly complex fiber networks.

The following work flow is applied. First of all, the single fibers which form the compound are geometrically analyzed. Furthermore, highly resolved three-dimensional computer tomography (μCT) images of wood fiber based insulating materials are generated. From these geometrical characterizations the fiber network and the pore volume distribution are evaluated.

In a second step based on these characterizations virtual realizations of the materials are generated. Subsequently, the microstructural simulation of the heat transfer in these virtual representation is carried out and compared to experiments. An advantage of this microstructural simulation technique is that as input only the conductivity of the wood fibers is required.

Studies on the influence of different process parameters as fiber length distribution, fiber orientation and raw density are possible by generation of appropriate virtual microstructures. Furthermore, effective (global) as well as local quantities are evaluated. Therefore, this virtual material testing approach allows the prediction and optimization of insulating material without extensive trial and error approaches.

The presented simulations are prepared by using the commercial software tool Geodict [2] and the fast microstructure Solver FeelMath [2]. This efficient solver directly operates on voxel images and thus no effortful generation and storage of meshes is required. Thus, very large microstructures, either virtually generated or directly obtained from μCT images, can be simulated fast and memory efficient.

References:

Acceptance of Terms and Conditions:
Click here to agree
The densities of Minkowski functionals (volume, surface, mean curvature and total curvature) represent a complete set of independent global microstructural descriptors [1-3], as a consequence of Hadwiger’s characterization theorem [4]. Similar to correlation functions [5, 6] they offer a systematic and principally automatizable approach for the quantitative description of microstructures, but unlike the latter they form a complete set of simple parameters that are readily determined on real microstructures and, if appropriately implemented into microstructure-property relations, could provide more accurate predictions of effective properties than micromechanical bounds or model predictions based on volume fractions alone. In this contribution we present examples of the application of Minkowski-functional-based global descriptors for the quantitative description of porous ceramics. We show that, apart from the porosity (pore volume fraction) and mean chord length (based on the phase-specific surface density) also a generalized Jeffries size (based on the mean curvature integral density) can be determined from planar sections [1,7,8]. The correlation between these two independent size measures is analyzed and the average pore size thus determined is compared to the characteristic values (quantiles and mean values) extracted from pore size distributions (number- and volume-weighted) determined via microscopic image analysis, after correcting for the random section problem (Wicksell’s problem [9]) via appropriate transformation matrices [10]. Moreover, it is shown how the 3D Euler characteristic can be determined on (appropriately binarized) serial sections of spatial images (obtained by X-ray computed tomography).

References:


Acceptance of Terms and Conditions:

Click here to agree

Invited 1 (Room C) - Leonhard Ganzer / 1121
Microvisual Studies of Fluid Flow in Enhanced Oil Recovery Processes

Leonhard Ganzer1

1 Clausthal University of Technology

Corresponding Author(s): leonhard.ganzer@tu-clausthal.de

The complex fluid flow processes occurring during EOR methods are difficult to implement in numerical modeling. Therefore, this presentation aims to share some light on experimental results from microfluidics studies conducted for various multi-phase fluid displacement processes with a focus on chemical EOR methods using brine, polymer-, alkaline- and surfactant-solutions. A wide range of important fluid-fluid and fluid-grain interactions can be observed and characterized using the visual outcomes of the experiments. Upscaling to continuum-scale reservoir simulation still poses challenges, but the microvisual studies can support these. Applications ranging from water injection all the way to ultra-low interfacial tension surfactant displacement processes will be shown including some numerical simulation results of the experiments.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-F / 942

Mineralogical and transport controls on the evolution of porous media texture

Sergi Molins1 ; David Trebotich1 ; Carl SteefelNone

1 Lawrence Berkeley National Laboratory

Corresponding Author(s): smolins@lbl.gov

Understanding the evolution of porous media is essential for many subsurface energy applications, including subsurface storage, shale gas production, fracking, CO2 sequestration, nuclear waste storage, and geothermal energy extraction. Both mineral composition and the initial pore structure of the medium play a significant role in this evolution. Conventional Darcy-scale models treat porous media as a continuum. This approach requires the assumption of well-mixed conditions inside the pore space as well as the use of mechanistic relationships between bulk parameters as the porous medium evolves (e.g. porosity-permeability, porosity-tortuosity). More recently, pore-scale models along with advanced characterization techniques have allowed for accurate simulations of flow and reactive transport within the pore space. Here we use pore scale modeling to study the evolution of mineralogically and physically heterogeneous porous media as a result of mineral dissolution. We consider scenarios associated with CO2 sequestration focusing on the dissolution of carbonate minerals under a range of flow conditions in granular and fractured domains. For this purpose, a pore-scale flow and reactive transport model is developed that explicitly tracks mineral surfaces as they evolve using a direct numerical simulation approach.

Simulations of dissolution in single-mineral domains provide insights into the transport controls at the pore scale, while the simulation of a fracture surface composed of bands of faster-dissolving calcite and slower-dissolving dolomite provides insights into the mineralogical controls on evolution. Transport-limited conditions at the grain-pack scale may result in unstable evolution, a situation in which dissolution is focused in a fast-flowing, fast-dissolving path. Due to increasing velocities, the evolution in these regions is like that observed under conditions closer to strict surface control at the pore scale. That is, grains evolve to have oblong shapes with their long dimensions aligning with the local flow directions. Another example of an evolving reactive transport regime that affects local rates is seen in the evolution of the fracture surface. As calcite dissolves, the diffusive
length between the fracture flow path and the receding calcite surfaces increases. Thus, the calcite dissolution reaction becomes increasingly limited by diffusion.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-B / 815

Mitigation of arsenic mass poisoning

Ian Griffiths1; Sourav Mondal1; Raka Mondal1; Sirshendu De2

1 University of Oxford
2 IIT Kharagpur

Corresponding Author(s): ian.griffiths@ymail.com

Arsenic is one among the most hazardous contaminants present in drinking water sources. Recent increases in agricultural growth and extensive use of fertilisers in India and Bangladesh have led to the release of naturally occurring arsenic from the rocks and earth’s crust, creating a major public health issue in these countries. A novel technology has been recently developed that uses naturally abundant laterite soil to filter arsenic, and now provides filtered water to more than 5000 people. To upscale this technology and enable it to realise its full potential requires an understanding of how the filter lifetime depends on the operating regime e.g., the required flow rate, contaminant concentration and filter size. In this poster we show the mathematical model we have been developing that characterises the arsenic removal that avoids the need for time-consuming experiments. The model is reduced to a system that can be described by a single dimensionless parameter, the filter rating, which characterises the entire filter behaviour. The resulting model enables efficient parameter sweeps to be performed that predict how the lifetime of a filter in a specified role, such as a family home, school or community filter.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-B / 518

Mixed methods for 1D-3D coupled flow models in porous media

Ingeborg Gåseby Gjerde1; Jan Nordbotten1; Kundan Kumar1

1 University of Bergen

Corresponding Author(s): ingeborg.gjerde@uib.no

The physical processes governing flow and transport in porous media span a wide array of spatial scales. Furthermore, in many applications it would be computationally intractable to resolve each scale of interest. To still capture the effects of the smaller-scale processes, one option is to couple together models of different dimensionality. In e.g. vascularized tissue and root networks, the arteries and roots have negligible radius compared to their own lengths. They can therefore be viewed as 1D inclusions embedded in the 3D domain, and the system modeled using a coupled 1D-3D flow model.
We consider the use of mixed finite element methods to solve 1D-3D coupled porous media flow problems. Due to the high dimensional gap between the models, the solutions of this system will be singular to the point of eluding the standard $H^1$ framework. Existence proofs and convergence rates therefore require special consideration. In this talk, we will use weighted Sobolev spaces to prove the existence of a solution to both continuous and discrete mixed formulation. We then perform a numerical analysis of the problem and present simulation results.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 526

Mixed methods for coupled 1D-3D flow models in porous media

Jan Nordbotten 1 ; Kundan Kumar 1 ; Ingeborg Gåseby Gjerde 1

1 University of Bergen

Corresponding Author(s): ingeborg.gjerde@uib.no

The physical processes governing flow and transport in porous media span a wide array of spatial scales. Furthermore, in many applications it would be computationally intractable to resolve each scale of interest. To still capture the effects of the smaller-scale processes, one option is to couple together models of different dimensionality. In e.g. vascularized tissue and root networks, the arteries and roots have negligible radius compared to their own lengths. They can therefore be viewed as 1D inclusions embedded in the 3D domain, and the system modeled using a coupled 1D-3D flow model.

This poster presents an analysis of the mixed finite element method applied to coupled 1D-3D porous media flow problems. Due to the high dimensional gap, the solutions will be singular around the inclusion. As a result, the problem eludes the standard $H^1$ framework, and weighted Sobolev spaces must be employed instead. We prove existence of a solution to the continuous and discrete model, obtain weighted error rates for the method, and present simulation results.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-B / 93

Mixed-dimension models for network flow in biological systems

Tobias Koepl 1 ; Rainer Helmig 1 ; Timo Koch 1

1 University of Stuttgart

Corresponding Author(s): tobias.koepl@iws.uni-stuttgart.de

Hierarchical network structures occur in many biological systems, since they are responsible for the transport of fluids, nutrients or oxygen. Such a network structure is, for example, the blood vessel
network supplying organs with oxygenated blood or removing metabolic waste from the tissue. A further example is the root network of a plant, ensuring the plant’s water supply.

One way to obtain a realistic mathematical model for such processes is based on a decomposition approach. Thereby, the network structure is separated from the surrounding medium and different models are assigned to both domains. Often, the surrounding medium (e.g. tissue or soil) is considered a three-dimensional (3D) porous medium. To decrease computational costs while maintaining a certain degree of accuracy, flow and transport processes within the networks are modeled by one-dimensional (1D) PDE-systems based on cross-section averaged quantities. A coupling of the network and the porous medium model is achieved by first averaging the 3D quantities and projecting them onto the 1D network structure. As a next step, a transfer function based on the difference of the averaged 3D and 1D quantities is computed and incorporated into the source/sink terms of the corresponding models. The source term of the 3D problem exhibits a Dirac measure concentrated on the 1D network.

In this talk we present several application areas for this kind of coupling concepts. Furthermore, we are concerned with the numerical analysis of PDE systems arising in the context of this model concept. In particular, it is investigated how the Dirac source terms and averaging operators affect the convergence behavior of standard finite element methods. Therefore, elliptic model problems with Dirac source terms and averaging operators are investigated. Our theoretical results are confirmed by numerical tests.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 186

Mixed-dimensional modeling of the brain’s waterscape

Cécile Daversin-Catty\(^1\), Marie E. Rognes\(^\dagger\)

\(^\dagger\) Simula Research Laboratory

Corresponding Author(s): cecile@simula.no

The clearance of the metabolic waste in the body is handled by the lymphatic system. Except in the brain, which appears to be the only organ devoid of lymphatic channels. Indeed, the mechanisms underlying the clearance processes of the brain are still unknown, and the topic sparks debate and controversy. What is clear however, is that dysfunction of cerebral metabolic waste clearance is associated with neurodegenerative disorders such as Alzheimer’s disease.

The term the brain’s waterscape refers to the circulation, flow and exchange of tissue fluid and transport of solutes through the brain. While these processes are not fully understood yet, most hypotheses point out the major role of the cerebral blood vessels and possibly paravascular spaces. We propose to investigate these processes using a mathematical approach based on coupled mixed-dimensional models mimicking the vasculature and paravascularity as topologically one-dimensional structures embedded in a three-dimensional porous medium.

This poster presents a mixed-dimensional model dedicated to the mesoscale-macroascale interaction between the brain tissue, the vasculature and the paravascularity, aiming at gaining new insight into the waste clearance process of the brain. The formulation and well-posedness of this model will rely on non-standard techniques such as weighted Sobolev spaces and non-local averaging operators used in\(^\ddagger\).

References:

Acceptance of Terms and Conditions:
Parallel 8-B / 185

**Mixed-dimensional models of the brain’s waterscape with FEniCS**

Cécile Daversin-Catty\(^1\) ; Marie E. Rognes\(^1\)

\(^1\) *Simula Research Laboratory*

**Corresponding Author(s):** cecile@simula.no

The clearance of the metabolic waste in the body is handled by the lymphatic system. Except in the brain, which appears to be the only organ devoid of lymphatic channels. Indeed, the mechanisms underlying the clearance processes of the brain are still unknown, and the topic sparks debate and controversy. What is clear however, is that dysfunction of cerebral metabolic waste clearance is associated with neurodegenerative disorders such as Alzheimer’s disease.

The term the brain’s waterscape refers to the circulation, flow and exchange of tissue fluid and transport of solutes through the brain. While these processes are not fully understood yet, most hypotheses point out the major role of the cerebral blood vessels and possibly paravascular spaces. We propose to investigate these processes using a mathematical approach based on coupled mixed-dimensional models mimicking the vasculature and paravascular as topologically one-dimensional structures embedded in a three-dimensional porous medium.

This talk introduces a mixed-dimensional model dedicated to the interaction between the brain tissue, the vasculature and the paravascular, aiming at gaining new insight into the waste clearance process of the brain. The development of this model relies on the FEniCS open-source finite element library\(^2\). We will also present dedicated features developed in a wider context of automating mixed-dimensional finite element in FEniCS. The introduced tools will be illustrated by concrete examples of applications in biomedicine in general and for the brain’s waterscape in particular.

**References:**


Click here to agree

---

Poster 1 / 918

**Mixing and reactions: The case of Taylor dispersion in a tube**

**Author(s):** Brian Wood\(^1\)

**Co-author(s):** Taghizadeh Ehsan \(^1\)

\(^1\) *Oregon State University*

**Corresponding Author(s):** brian.wood@oregonstate.edu

The progression of reactions in systems where mixing occurs has been the subject of investigation for decades; however, there is still much that is unknown about such systems. One area of particular interest to us is the influence of the initial configuration of a system as it evolves in time. Many (if not most) investigations of mixing are formulated at the long time limit, which requires that a certain amount of relaxation of the system has occurred. Although this is an interesting regime that has relevant to, for example, reactions occurring in the subsurface, it does not describe the initial phases of mixing well.
In this work, we examine how the initial configuration of a system can influence the mixing and reaction process evolution. Such early time conditions have relevance to many systems. For example, in industrial processes the basic design constraints of mixing facilities essentially requires that the mixing regime is dominated by early time behavior (e.g., the effective reaction rate for multi-component injections into tubular, packed bed, or fluidized bed reactors would all generally depend strongly on the initial configuration of the chemicals introduced).

Because mixing is exceptionally complex, we have chosen to examine a two-component mixing and reaction process within a tubular reactor. This choice is motivated in part by the simplifications that this geometry allows, and in part because of recent successes we have had in better understanding the early time dispersion process (pre-asymptotic Taylor dispersion) in such systems. The results of this work will focus primarily upon (1) development of the effective mass transport equations (resulting in an explicit representation of convection, effective dispersion, and the effective reaction rate), and (2) presentation of a closure scheme for this problem, and an prediction of the effective rate of reaction via numerical computations. In particular, we will discuss the need to search for effective empirical dynamical scaling laws even in the presence of a fully-predictive theory. The need for empirical models arises because, in this particular case, the process of upscaling does not reduce the complexity of the problem to the extent that would be the most useful for applications.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-A / 881

Mixing effects in agrochemical biodegradation networks in variably saturated soils

Giovanni Porta¹ ; Daniele la Cecilia² ; Fiona Tang² ; Monica Riva³ ; Federico Maggi²

¹ Dept. of Civil and Environmental Engineering, Politecnico di Milano
² School of Civil Engineering, The University of Sydney
³ Dipartimento di Ingegneria Civile e Ambientale (DICA), Politecnico di Milano

Corresponding Author(s): giovanni.porta@polimi.it

Few current bioreactive transport solvers currently provide a comprehensive mechanistic description of biogeochemical cycles and allow easy integration of all the involved processes, including flow in variably saturated media, solute transport and kinetic/equilibrium biochemical reactions. The parameterization of these processes is particularly challenging since our knowledge of model parameters and of their spatial heterogeneity is typically incomplete. Therefore, it is crucial to study the impact of each process and related parameters uncertainty in the outputs of interest.

In this communication, we consider reaction networks describing biochemical degradation of herbicides, atrazine and glyphosate (la Cecilia and Maggi, 2017a, 2017b). In particular, we quantify the degradation potential and accumulation of toxic substances and we study the biomass and ecological structure dynamics in soil and groundwater. Our discussion encompassed the assessment of model outputs sensitivity on the identified model structure and related parameters. We focus on the effects of local mixing, which entails the full characterization of spatial and temporal fluctuations of solutes concentration within the time-space domain. We frame these analyses in terms of dimensionless parameters describing the integrated processes of interest, i.e., fluid flow, solute transport, and biogeochemical reactions and we identify global trends and statistical indicators to characterize the system at steady state. This work will address system nonlinearities linked to the interplay of diverse processes with the aim of increasing our understanding of dominant mechanisms involved in agrochemicals bioreactive transport.

References:

Parallel 5-C / 506

Model-based interpretation of tracer tests in fractured limestone and clayey till

Author(s): Klaus Mostad
Co-author(s): Peter R. Jorgensen ²; Rasmus Thalund-Hansen ¹; Mette M. Broholm ¹; Poul L. Bjerg ¹; Massimo Rolle ¹

¹ Technical University of Denmark
² PJ-Bluetech ApS

Corresponding Author(s): klmos@env.dtu.dk

The importance of fracture flow and matrix diffusion was investigated in two different fractured geometries: limestone and clayey till. Natural- and forced-gradient tracer tests were designed and conducted to analyze the transport behavior in the two fractured media and to investigate the required model complexity for the simulation of solute transport. A discrete-fracture model was employed to plan and interpret the tracer tests in the two different geologic settings. We present results from:

1) A pumping test combined with depth-discrete tracer tests in fractured limestone using fluorescent and ionic tracers with different diffusion properties
2) An infiltration tracer test in clayey till using the color tracer brilliant blue to identify the major transport pathways

The pumping and tracer tests and geologic investigations showed that the fractured limestone is highly permeable with fractures dominating the primary solute transport. The conductivity of major fractures has a strong contrast to the limestone matrix. The diffusive interaction between fractures and matrix was revealed by significant tailing in the tracer breakthrough curves at the pumping well. The observed behavior demonstrated the importance of including fracture flow and transport in the modeling of solute transport at fractured limestone sites. The simultaneous injection of multiple tracers with different diffusion properties facilitated the analysis of compound-specific fracture-matrix interactions.

The infiltration tracer test in the clayey till was performed in a large-scale excavation at an agricultural field site to identify the major transport pathways and to assess groundwater vulnerability to pesticides leaching. The tracer experiment revealed low fracture conductivities. Despite many fractures were filled with precipitate and only few of the visible fractures were hydraulically active, they were still major transport pathways for the applied tracer. The infiltration depth and the diffusion length into the matrix were used to infer hydraulic apertures of the fractures. These are compared to the apertures determined in large undisturbed column tests on the same soil material. The infiltration tracer test allowed to identify the hydraulically active fractures. These were incorporated as a 3D fracture network into a 3D model representing these main preferential flow and transport paths as well as the exchange with the clayey till matrix.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-A / 64
Modeling CO2 Storage in Fractured Reservoirs: Fracture-Matrix Interactions of Supercritical and Dissolved CO2

Quanlin ZHOU¹ ; Curtis M. Oldenburg¹ ; Jens T. Birkholzer¹

¹ Lawrence Berkeley National Laboratory

Corresponding Author(s): qzhou@lbl.gov

The injection and storage of supercritical CO2 (scCO2) have been conducted in fractured sandstone reservoirs at In Salah, Algeria and Snøhvit, Norway, and planned in fractured sandstone, carbonate, and dolomite reservoirs at Longyearbyen, Norway, Hontomin, Spain, and Kevin Dome, USA, respectively, with matrix permeability varying from 0.01 to 60 md. For densely fractured reservoirs with low matrix permeability (e.g., at Longyearbyen, Norway), injected scCO2 can dissolve into the resident brine at fracture-matrix interfaces and the dissolved CO2 (dsCO2) can diffuse into the rock matrix making solubility trapping the dominant trapping mechanism. For fractured reservoirs with intermediate matrix permeability (e.g., at In Salah, Algeria), the storage of scCO2 in the rock matrix dominates with strong fracture-matrix interactions observed through field monitoring at In Salah. We developed a comprehensive conceptual model for enhanced CO2 storage to account for global migration of scCO2 in the fracture continuum, local storage of scCO2 and dsCO2 in the matrix continuum, driving forces for scCO2 invasion and dsCO2 diffusion from fractures, and brine outflow through connected matrix blocks.

For the dominant matrix scCO2 storage, we developed high-resolution fracture-matrix models for individual matrix blocks, homogeneous columns of fractures and matrix blocks, and heterogeneous REVs consisting of multiple columns of matrix blocks with varying flow properties and sizes. The multiscale modeling results show that the equilibrium efficiency of local scCO2 storage strongly depends on matrix entry capillary pressure, matrix-matrix connectivity, and reservoir thickness, while dynamic efficiency and transfer function are also sensitive to fracture spacing and matrix flow properties. The transfer functions calculated for various REVs were used along with reservoir-scale dynamics of scCO2 plume flow in fractures, showing that the preferential migration of scCO2 through fractures is coupled with bulk dsCO2 storage in the rock matrix that in turn retards the scCO2 fracture plume. The bulk matrix storage is mainly driven by buoyancy between fracture scCO2 and matrix brine and facilitated by matrix-matrix connectivity that allows displaced brine to outflow, enabling the rock matrix to act like an open system. Conventional dual-continuum models cannot capture these processes because they model isolated matrix blocks with no capillary continuity, thereby underestimating storage efficiency.

For the dominant matrix dsCO2 storage, we developed the unified-form equations of diffusive flux of dsCO2 into brine-bearing matrix blocks of varying shapes (i.e., spheres, cylinders, slabs, squares, cubes, rectangles, and rectangular parallelepipeds) and sizes (Zhou et al., 2017a, b). We then applied the flux equations to a fractured reservoir with various scenarios of matrix blocks by assuming 1-D and 2-D radial scCO2 flow in fractures and by using diffusion of dsCO2 from fracture-matrix interfaces into matrix blocks as the sink for scCO2 in fractures. For each scenario, the dynamic dsCO2 plume with different mass fraction was produced analytically, showing that solubility trapping is significant in fractured reservoirs with low matrix permeability and small fracture spacing.

References:


Click here to agree

Parallel 8-C / 898
Modeling Energized Fluids Fracturing with Phase Field Method

Author(s): Mohamad Jammoul

Co-author(s): Benjamin Ganis, Mary Wheeler, Sanghyun Lee

1 Center for Subsurface Modeling, University of Texas at Austin
2 The University of Texas at Austin
3 Florida State University

Corresponding Author(s): jammoul@utexas.edu

The use of energized fluids in hydraulic fracturing helps minimize formation damage and enhance well productivity especially in water sensitive reservoirs. Many current fracking simulators use single phase and incompressible flow assumptions to model the fracturing fluids. The thermal and compositional effects of using energized fluids on fracture topology are neglected by such simulators. A computational framework has been developed to model the fracture propagation resulting from energized fluids fracturing. The framework couples a phase field fracture propagation software with a compositional reservoir simulator. It models the flow of multiphase multicomponent fluids in the fractures and in the reservoir. Numerical tests were conducted to emphasize the effect of fluid compressibility and composition on fracture propagation and geometry.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-B / 976

Modeling Soil Water Retention Curve under Non- Isothermal Conditions

Farshid Vahedifard, Toan Cao, Sannith Thota, Ehsan Ghazanfari

1 Mississippi State University
2 University of Vermont

Corresponding Author(s): farshid@cee.msstate.edu

Several emerging problems in geotechnical and geoenvironmental engineering pose multi-physics problems involving non-isothermal processes in unsaturated soils. Properly studying these problems requires the development of models for the Soil Water Retention Curve (SWRC) to describe the constitutive behavior of unsaturated soils under non-isothermal conditions. This study aims to develop analytical expressions of non-isothermal SWRCs. Closed-form expressions are presented to consider the effects of temperature on adsorption and matric suction in unsaturated soils. The formulation for the non-isothermal matric suction accounts for the effects of temperature on the surface tension, soil-water contact angle, and adsorption by the enthalpy of immersion per unit area. The formulations are then employed to extend several existing isothermal SWRCs to non-isothermal conditions. The extended SWRC models are used in a parametric study to examine changes in adsorbed water, capillary water and total water content versus matric suction for Ottawa sand and Wyoming bentonite subjected to several temperatures ranging from 25 °C to 100 °C. The results show that temperature can have significant effects on SWRCs, depending upon the soil type and range of temperature. Further, the results obtained from the proposed formulations are compared against three independent laboratory test results and very good agreement is observed with the tests conducted on sand, silt, and clay under different temperatures. The proposed formulations can be readily incorporated into analytical solutions and numerical simulations of thermo-hydro-mechanical models of unsaturated soils. The findings of the study can facilitate using numerical models to simulate various non-isothermal applications involving geo-energy systems and soil-atmospheric interaction problems.
Parallel 1-F / 492

Modeling Wettability Alteration Induced by Asphaltene and Fluid Behaviors at the Interface

Jiajun He¹ ; Cesar Mantilla¹ ; Birol Dindoruk¹

¹ Shell Int. E&P

Corresponding Author(s): jiajun.he@shell.com

Wettability is a paramount factor in multiphase flow through porous media. The preference of the rock mineral surface to oil or brine determines fundamental flow functions in reservoir engineering like irreducible saturations, critical saturations, relative permeability and capillary pressure. Its implications affect all processes in oil and gas recovery, from primary production, waterflooding, to enhanced oil recovery. Except for a few specialized cases (low salinity waterflooding), reservoir modeling is done without considering wettability alteration during these processes.

There is experimental evidence in the literature that the presence of asphaltene can alter rock wettability towards more oil-wet. However, on one hand, modeling wettability of porous rocks is difficult because many complex factors interact in the system, which cannot be considered independently. Even a perfect independent description of rock, and two fluid phases is not sufficient to accurately model the wettability of a rock. On the other hand, asphaltenes (the heaviest, most polar component of crude oils) are a class of complex, not well-defined molecules, with behaviors that affect the water/oil/solid interactions and hence wettability. At the current state of the art, there is no comprehensive model that can predict wettability, not even without the complexity of asphaltene behaviors.

We present here a model based on the DLVO theory with fundamental forces in the equilibrium of a flat solid surface with two fluids (brine/oil, wetting/non-wetting) at nanoscopic scale. The force equilibrium results in a macroscopic contact angle formed by a drop of oil over a thin film of brine over a solid surface. With the inputs of physical parameters, such as asphaltene content, oil/water interfacial tension, electric surface potentials, and brine composition, the developed model is able to predict contact angle alteration as function of changes in any of the inputs.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-C / 356

Modeling fracture reactivation in a mixed dimensional setting: Friction models and numerical challenges

Author(s): Runar Berge¹
Co-author(s): Inga Berre ¹ ; Eirik Keilegavlen ⁱ ; Jan Nordbotten ⁱ

¹ University of Bergen
Corresponding Author(s): runar.berge@uib.no

Reactivation of fractures is a strongly coupled problem involving disparate physical processes such as fluid flow, temperature and rock deformation. We present a coupled mixed dimensional model, where the main focus is on the deformation of fractures. We will discuss numerical solutions of friction models for the reactivation of pre-existing fracture networks, and the treatment of the non-linearities introduced by the slip. Numerical examples include a 3D fracture network inspired by realistic data.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-C / 926

Modeling hydraulic fracturing using a vectorized 3D implementation of XFEM

Ehsan Haghighat\textsuperscript{None}; Ruben Juanes\textsuperscript{1}

\textsuperscript{1} MIT

Corresponding Author(s): ehsan@mit.edu

Hydraulic fracturing is a subsurface stimulation technology that has been deployed at a massive scale in North America, and made it possible to produce hydrocarbons from low-permeability rocks, like oil shales and gas shales, which traditionally had been considered uneconomical. Despite this large-scale deployment, our understanding of the physics and controlling parameters in hydraulic fracturing is still very limited. One of the fundamental challenges is the ability to describe the interaction of rock tensile failure of an advancing fracture with the network of intersecting pre-existing fractures and cracks in the rock. Such interaction results in extension and coalition of initial cracks, and is wildly different from the well-understood process of the propagation by fluid injection of a smooth penny-shaped crack in a homogeneous porous medium.

From a traditional computational modeling standpoint, capturing fracture generation, growth and coalescence requires that each possible location of a fracture be added to the geometry and meshing process. As a result, this entails that the coupled flow-geomechanics equations be solved on an evolving unstructured mesh that dynamically adapts to each fracture zone—a computationally demanding, and poorly-scalable, approach.

Here, we present an approach to incorporate discrete fractures in the model, implicitly, through the Extended Finite Element Method (XFEM)\textsuperscript{[2]}. In this framework, the discontinuity is modeled by enriching the basis functions so that they can reproduce the discontinuous deformation along and across the surface of discontinuity. Use of XFEM for modeling hydraulic fracking was proposed a long time ago for two-dimensional problems [2], but its applicability for real-case three dimensional cases has not been addressed.

In our work, the geometry of each fracture is incorporated implicitly through a level-set technique [3]. A multi-grid level-set discretization is proposed and implemented to accurately regenerate the complexity of the fracture’s geometry without significant computational effort. We then use this representation to regenerate the enrichment functions. Here, we propose a new implementation for XFEM that is fully vectorized and hence very efficient to perform three-dimensional studies. We validate our XFEM model first by comparing with simulations using contact elements. We then present representative simulations with multiple fractures to show the capability of the framework. We demonstrate that this framework is well suited for optimization and inverse analysis, which often requires running a large ensemble of simulations.

References:
Parallel 9-C / 681

Modeling induced seismicity with coupled poroelasticity on discrete fracture networks with evolving hydraulic diffusivity and Mohr-Coulomb failure

Daniel Birdsell¹; Harihar Rajaram²; Satish Karra³

¹ University of Colorado, Boulder

Corresponding Author(s): daniel.birdsell@colorado.edu

Injection-induced seismicity (IIS) depends on pore pressure, in-situ stress state, and fault orientation; generally occurs in basement rock that contains fractures and faults; and moves away from the injection well as a nonlinear diffusion process. Therefore to numerically model IIS, a code should incorporate coupled flow and geomechanics, the presence of fractures and faults, and the capability for hydraulic diffusivity to evolve with effective stress and failure history. We use DFNWorks and a novel hybrid equivalent porous medium/discrete fracture network approach to generate and map fracture networks to a continuum grid where the fully coupled poroelastic equations are solved by PFLOTRAN. Hydraulic diffusivity has different constitutive relationships for fracture and matrix grid cells, and the seismic cloud can be tracked based on a Mohr-Coulomb failure calculation on each fracture. We discuss details and challenges in code development, including how the Bandis model can be used to calculate hydraulic diffusivity and stiffness for fractures within this framework. We apply our model to understand IIS at Greeley, CO and Paradox Valley, CO. The computational tools presented here can be applied to understand IIS, nuclear waste disposal, carbon sequestration, unconventional oil and gas production, and groundwater remediation.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-C / 689

Modeling nonlinear diffusion in fractured rock with deformable fractures and applications to injection induced seismicity

Ryan Haagenson¹; Harihar Rajaram²; Satish Karra³

¹ University of Colorado
² University of Colorado, Boulder
³ Los Alamos National Laboratory

Corresponding Author(s): ryan.haagenson@colorado.edu

In many applications such as geothermal energy, geological carbon sequestration, unconventional gas recovery, and injection induced seismicity (IIS), there is a need to model flow and transport phenomena in fractured rock. In fractured rock, the hydraulic and mechanical properties of the
fractures are extremely sensitive to fluid pressure and other perturbations. Although the general problem of hydromechanical coupling in fractured rock requires a simultaneously coupled solution of the pressure and stress fields, a partially uncoupled solution employing pressure-dependent fracture properties (with a time-invariant stress field) is still insightful. Here we present a model for hydromechanical coupling in fractured rock, implemented within the general-purpose finite element solver Fenics. The model allows representation of a discrete fracture network (DFN) within a rock mass. Fracture aperture and permeability are allowed to vary with fluid pressure, according to the Bandis constitutive model. Fracture permeability is also allowed to change due to slip events. Pressure diffusion is permitted in the fractures and rock matrix, including hydraulic interactions between them. The model can handle both incompressible and compressible fluids.

We present applications of the model to IIS, interpretation of hydraulic tests in fractured rock, and evaluate concepts such as effective storativity and generalized radial flow dimension. For IIS in particular, we attempt to replicate a seismic cloud dataset collected in Greeley, CO – providing insights into how the DFN structure effects the propagation of pressure increases throughout a fractured formation, leading to certain spatial-temporal patterns in induced seismic events. Using a frozen background stress field, seismic events are identified using the Mohr-Coulomb failure criteria. This approach to modeling pressure diffusion in the context of IIS improves over uncoupled approaches that typically only model diffusion (most commonly linear diffusion, with some previous works allowing for nonlinear diffusion) in equivalent porous continua. We also revisit other seismic cloud datasets to further explore relationships between DFN structure and seismic clouds.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-A / 404

Modeling porous medium modification through induced calcium carbonate precipitation

Author(s): Johannes Hommel

Co-author(s): Adrienne Phillips ; Robin Gerlach ; Al Cunningham ; Rainer Helmig ; Holger Class

1 University of Stuttgart
2 Montana State University
3 Center for Biofilm Engineering, Montana State University

Corresponding Author(s): johannes.hommen@iws.uni-stuttgart.de

Fluid storage in the subsurface is important to reduce climate change (sequestration of CO2) or for energy storage (CH4, H2) to cope with the intermittent, unpredictable production of renewable sources like wind and solar. However, the fluids have the potential to leak through damaged cap rocks or wellbores. One method to remediate these problems is inducing calcium carbonate precipitation (ICP). Currently, most applications of ICP rely on urea hydrolysis by microbes (MICP) to promote precipitation within the porous media. However, precipitation may also be induced by injection of extracted or plant-based sources of the enzyme urease (EICP) or at elevated temperatures (TICP). The applicability of a certain method of ICP is largely determined by the depth below ground surface and the local geothermal gradient. MICP has been demonstrated to have immense potential to seal leakage pathways, even at field scale [1] but is only effective within a limited temperature range, as it relies on the activity of living bacterial cells. As a consequence, the other ICP methods EICP and TICP have to be developed and demonstrated in the field. To assist experimental investigations on EICP and TICP, a previously developed numerical model for MICP [2,3] is generalized and adapted for the new precipitation-inducing processes. As the models are intended for the use in predicting the leakage mitigation for subsurface gas storage, they account for two-phase flow. Additionally, a variety of different components and processes are necessary to describe ICP, the specific number of components and processes being dependent on the precipitation-inducing process. All models are implemented in the open-source simulator DuMuX [4]. The primary variables solved are the aqueous-phase pressure, mole fractions of each component in the water phase, temperature, and,
for the solid phases, the volume fractions. The mass balance equations are solved fully implicitly and are coupled through the source and sink terms due to the reactions. The new kinetic rate equations for the developed EIC and TIC models were fitted to experimental data obtained from batch experiments at Montana State University. The porosity and permeability reduction due to calcium carbonate precipitation and accumulation of biomass or enzyme are accounted for by updating the porosity using the volume fractions of the solid phases and for the permeability by using the updated porosity and a Verma-Pruess-type relation [5]. The new models for EIC and TIC will be calibrated and validated using column experiment data, similarly to the procedure outlined in [3], which will then be used to determine the optimal mineralization method and injection strategy for given boundary conditions.

References:

Click here to agree

Parallel 1-A / 193

Modeling the dissolution-driven convection as a Rayleigh-Benard problem

Layachi Hadji¹

¹ The University of Alabama

Corresponding Author(s): lhadji@ua.edu

We examine the linear and weakly nonlinear stability analyses of the dissolution-driven convection induced by the sequestration of carbon dioxide in a geological formation. The mathematical model consists of Darcy’s equation, the conservation of mass and the conservation of solute equations. The model accounts for anisotropy in both carbon diffusion and permeability which is modeled by a decaying exponential function of depth. The presence of a first order reaction between the carbon-rich brine and host mineralogy is also included. We prescribe either Neumann or Dirichlet boundary condition for the concentration of carbon dioxide at the rigid upper and lower walls that bound a layer of infinite horizontal extent. We consider a Rayleigh-Taylor-like base state consisting of a carbon-rich heavy layer overlying a carbon-free lighter layer and seek the critical thickness at which this configuration becomes unstable. With this approach, standard mathematical methods that were successfully used in the study of Rayleigh-Benard convection can be applied to this problem. We quantify the influence of carbon diffusion anisotropy, permeability dependence on depth and the presence of the chemical reaction on the threshold instability conditions and associated flow patterns using the classical normal modes approach. The critical Rayleigh number and corresponding wavenumber are found to be independent of the depth of the formation. The weakly nonlinear analysis is performed using long wavelength asymptotics, the validity of which is limited to small Damkohler numbers. We derive analytical expressions for the solute flux at the interface, the location of which corresponds to the minimum depth of the boundary layer at which instability sets in. We show that the interface acts as a sink leading to the formation of a self-organized exchange
between descending carbon-rich brine and ascending carbon free brine. Plots of the high order perturbation terms for the concentration successfully reproduce the fingering pattern that is typically observed in experiments and full numerical simulations. Using the derived interface flux conditions, we put forth differential equations for the time evolution of the upward migration of the interface as the dissolution process progresses. We solve for the terminal time when the interface reaches the top boundary thereby quantifying the time it takes for an initial amount of injected super-critical Carbon dioxide to be completely dissolved. We also consider the case where the interface migration is accompanied by interface deformations that conform to the convection pattern.

References:


Poster 3 / 262

Modelling approach and benchmark experiments for Nernst-Plank based transport, Coulombic interactions and geochemical reactions in saturated porous media

Author(s): Riccardo Sprocati 1
Co-author(s): Matteo Masi 1; Biao Jin 3; Muhammad Muniruzzaman 4; Massimo Rolle 1

1 Department of Environmental Engineering, Technical University of Denmark, Miljøvej, Building 115, 2800 Kgs. Lyngby, Denmark
2 Department of Energy, Systems, Territory, and Construction Engineering, University of Pisa, Via C.F. Gabbba 22, 56122 Pisa, Italy
3 State Key Laboratory of Organic Geochemistry, Guangzhou Institute of Geochemistry, 510640 Guangzhou, China
4 Geological Survey of Finland, Neulanienmittie 5, 70211 Kuopio, Finland

Corresponding Author(s): masro@env.dtu.dk

The transport of electrolytes in porous media is affected by physical, chemical and electrochemical processes. Coulombic interactions significantly influence the behavior of electrolyte plumes at different scales, not only in diffusion-dominated conditions but also in advection-dominated flow regimes [1-3]. To model the spatial behavior of charge-induced interactions in multi-dimensional homogeneous and heterogeneous domains, we propose a Nernst-Planck based modeling approach for conservative and reactive transport. The model is based on a coupling between COMSOL Multiphysics® and PhreeqRM [4]. Important features of the proposed approach include transport of chemical species and not of chemical components, the definition of physically and chemically heterogeneous domains and the implementation of electromigration as well as of the flux components arising from the activity coefficient gradients. The model has been benchmarked with numerical simulations in PHREEQC [5], analytical solutions and high-resolution experimental datasets in homogeneous and heterogenous setups for steady-state and transient conditions in different dimensions (1D, 2D and 3D). Fully three-dimensional experiments on multicomponent ionic transport were also performed in this study and were used to validate the proposed modeling approach. Simulations show an excellent agreement with the experimental and modeling benchmark problems, thus highlighting the potential of the Nernst-Planck based model for the evaluation of conservative and reactive multicomponent ionic transport.

References:

Acceptance of Terms and Conditions:
Click here to agree
Modelling of advective and capillary flows in sandstone cores during the injection of supercritical CO2

Laurent ANDRE¹ ; Mohamed AZAROUAL² ; Arnaud LASSIN²

¹ BRGM - ISTO
² BRGM

Corresponding Author(s): m.azaroual@brgm.fr

Numerical simulations of injection of CO2sc or of a mixture (aqueous solution + CO2sc) in sandstone cores were carried out. These preliminary numerical tests have twofold targets: i) helping for designing lab experiments and to anticipate the experimental behaviors of such complex systems and ii) to explore complex conditions (flow-pressure-temperature-salinity) that could not be easily achieved in laboratory experiments.

These 1D simulations were done using the numerical code TOUGH2 (Pruess et al., 1999), with the ECO2N module (Pruess, 2005). This code allows performing multiphasic reactive transport (THC) modelling considering gas-liquid equilibria and the possibility for halite to precipitate (according to thermodynamic equilibrium) with potential feedback on the petrophysical properties (k-phi) of the rock. During these simulations, the rock matrix is supposed to not react significantly (i.e., no dissolution of the sandstone at the scale of the simulation time).

To get closer to the experimental constraints, all THC simulations were done through cores the dimensions of which correspond to the actual samples used in lab tests. The hydrodynamic and petrophysical properties are those of a Vosges sandstone sample taken in a quarry in the East of France. The duration of the simulated injections is about 15 hours. In order to characterize the hydrodynamic and salt deposition processes in the core, a very fine mesh was set up: the core was divided into 75 cells of 1 mm thickness and of identical hydrodynamic properties. Initially, the core is saturated with NaCl-bearing brines (with salinity from 3 to 6 molal).

Among the various simulations performed, one corresponds to a low-pressure gradient, i.e., a low gas flow rate. The time needed to dry out the column is extremely long and the risk of clogging is important. Indeed, after the piston effect happens (flush of the most mobile water), water evaporation (i.e., water transfer into the CO2-rich fluid) is the only mechanism able to dry the porous medium. TOUGH2 allows modelling a capillary feedback (opposite to the advective flow of the CO2-rich phase), which maintains a quasi-stationary back-flow of the more concentrated brine toward the core entrance. Thus, the porosity close to the core inlet is continuously fed with brine, the evaporation of which provokes a massive precipitation of salt at the column inlet. Successive cycles of injection/stop further increase these risks by allowing brine flowing back towards the inlet of the core because of the re-distribution of fluids during the stop phases.

In conclusion, although the numerical code is devoted to simulations at the reservoir scale, it is possible to represent processes at small (centimeter) scales helping smart lab experiments. The advantage of the numerical approach is also to perform a large number of simulations to better determine the key processes and critical parameters and thus define the most relevant experimental tests to perform for more focused locks and mechanisms. The global methodology of these exploratory modeling will be presented at this minisymposium. The experimental results will be discussed and the relation “Flowrate-Pressure-Temperature” will be discussed regarding the injectivity of sandstone saline reservoirs.

References:

Acceptance of Terms and Conditions:

Click here to agree

Modification of wettability and interfacial tension by biosurfactant-producing bacteria for geologic carbon storage

Taehyung Park¹ ; Minkyung Jeon¹ ; Seunghiee Kim² ; Tae-Hyuk Kwon²

¹ Geological Survey of Korea
² Korea Research Institute of Geoscience and Technology
Injection of carbon dioxide (CO2) into deep geologic formations has been widely proposed as an effective way for the permanent storage of CO2. Modification of the interfacial properties of CO2 in minerals by using surfactant has been proposed aiming on increasing the mobility of CO2 through porous media. Surfactants are proven to effectively alter the interfacial tension and wettability in both CO2/water/mineral system, improving the displacement and sweep efficiencies of CO2 in porous media. In the meantime, biosurfactants have been drawing much attention as an alternative to the chemical surfactants for their biodegradability, ecological suitability and low toxicity. However, the question as to the extent of microbial alterations in fluid wettability and interfacial tension under reservoir pressure and temperature conditions still warrants further investigation. Therefore, this study investigated the role of lipopeptide biosurfactant on wettability and interfacial tension alterations in a CO2/brine/mineral system for different CO2 phases during the growth of thermotolerant and barotolerant bacteria, Bacillus subtilis, and the production of lipopeptide biosurfactant, surfactin. Quartz, mica and carbonate substrates were selected and used as representative minerals. While monitoring the changes in the interfacial tension and wettability with pH, fluid samples were acquired from the brine phase, and the concentrations of glucose, nitrate, ammonium and surfactin in the acquired samples were quantitatively assessed using various assays and spectroscopic methods. As a result of surfactin production by B. subtilis, we observed the reductions in interfacial tension and increases in contact angle at all tested cases. The concentration of surfactin and the rate of wettability alteration differed with the experimental conditions. The modification of CO2 wettability was the greatest for liquid CO2 while the least of modification was observed for gaseous CO2. The obtained results allow in-depth assessment of the feasibility of using biosurfactant-producing bacteria for effective geologic carbon storage practices.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-D / 899

Mogno – a high-throughput micro and nanotomography beamline at Sirius, the new Brazilian Synchrotron Light Source

Nathaly Lopes Archilha¹ ; Gabriel Schubert Ruiz Costa¹ ; Eduardo Xavier Miqueles¹ ; Harry Westfahl Jr.¹

¹ CNPEM

Corresponding Author(s): nathaly.archilha@lnls.br

The Brazilian Synchrotron Light Laboratory (LNLS) is currently engaged in the construction and development of Sirius, the largest and most complex scientific infrastructure ever built in Brazil and one of the first 4th-generation Synchrotron Light Sources in the World. Its ultra-low emittance (0.28 nm.rad) and high brightness will allow the execution of very competitive experiments, opening new perspectives for research in many different fields, including material science, nanoscience, physics, earth and environmental science.

Mogno is being designed to be a world-leading micro/nano imaging beamline focused towards multi-scale analysis (resolution ranging from hundreds of nanometers to dozens of micrometers) of the internal 3D structures of different materials and objects. The beamline will be primarily devoted and specialized in zoom-tomography, where a specimen can be studied at low and high-resolution. In parallel, Mogno competences will be extended to 4D imaging through in-situ experiments, which will allow the researchers to observe and quantify material responses during mechanical, thermal or chemical loadings, in real time. The goal is to obtain full resolution scan times in the order of 1 to 5 seconds. This can be achieved given the extremely high flux provided by a 3.2T bending magnet, the well design optical system and improvements in detection efficiency, as evident in direct
detection devices. Overall, all the processes (from robotic arms for sample exchanges, automatic alignment, data post-processing - reconstruction, segmentation and quantitative data analysis), are being optimized to make Mogno a high-throughput beamline.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-B / 660

Moisture-induced swelling of oil-painted linen canvas: experiments and modelling

Dominique Derome¹ ; Xiaohai Zhou¹ ; Robert Fischer²; Jan Carmeliët²

¹ Empa
² ETHZ

Corresponding Author(s): dominique.derome@empa.ch

Oil-painted linen canvas is a well-used art support system, used for more than five centuries, where the capacity of the canvas and its wood frame to absorb water is not only an issue of dimensional stability and modified material properties, but also of durability and damage for the stiff oil paint. In effect, as water molecules are adsorbed into the hydrophilic matrix in the plant cell walls, the induced fluid-solid interaction forces result in a swelling of the cell walls. Moisture-induced internal stresses highly influence the hygro-mechanical behavior of linen and wood as observed at the macroscale. Further, the interaction of the composite polymeric material, that is the layer S2 of wood and linen cell walls, with water is known to rearrange the internal structure, make it moisture sensitive and influence its physical properties, as demonstrated by fundamental molecular dynamics investigations.[1]

Such paintings may be exposed to daily or seasonal environmental variations in relative humidity, although most museums try to minimize such loads. The system of interest here is made of a linen canvas, a size layer, which is traditionally animal glue, a chalk-glue ground layer to flatten the substrate and an oil paint layer, incorporating diverse pigments. The canvas and the size used are hygroscopic, as the textile is made of flax fibers, which cell walls are a polymer-based (i.e. cellulose, hemicellulose and pectins) nanoporous material, while the glue is a protein-based material with subsequent loss of stiffness at high relative humidity. Both materials, and the wood frame, undergo significant swelling and shrinkage under moisture content variation. On the other hand, the oil layer is hydrophobic and dimensionally stable under varying moisture conditions, undergoing internal stress during movement of the base layer.

A multiscale experimental and modelling framework is developed to capture the phenomena of moisture transport, sorption and swelling. We present here the behavior of painted canvas samples undergoing changes in moisture content documented by laboratory X-ray tomography in order to better understand the coupled hygro-thermo-mechanical response of paintings as complex layered systems. The swelling of unrestrained small samples is captured, in terms at the yarn, textile and system scale. Accompanying this experiment, previous work has documented the sorption isotherms of the components of oil-painted canvas [2, 3]. With the moisture-induced swelling and the material properties documented adequately, a finite element model of the hygromechanical behavior of the layered system is then developed and used to identify risk associated with different environmental regimes.

Acknowledgement to contributions of Roel Hendricks, Stephan Hartmann and Stefan Carl.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-H / 764

Molecular Simulation Study of Swelling Clays

Arun Kumar Narayanan Nair¹ ; Shuyu Sun²

¹ KAUST, Saudi Arabia
² King Abdullah University of Science and Technology (KAUST)

Corresponding Author(s): arun.narayanannair@kaust.edu.sa

Grand canonical Monte Carlo and molecular dynamics simulations were applied to understand the molecular mechanism of species transport in clays. The variation of clay basal spacing as a function of relative humidity predicted based on the swelling free energy profiles was consistent with X-ray data. The hydration of clays shows the following well-known order: Mg²⁺ > Ca²⁺ > Sr²⁺ > Li⁺ > Na⁺ > K⁺. The diffusion of water and ions generally increases with relative humidity in all samples. Swelling due to H₂O intercalation processes could lead to permeability changes that directly impact successful storage of carbon dioxide. We observed a favorability of adsorption of CO₂ (or CH₄ to a lesser extent) by clays at intermediate preadsorbed water contents. At low pressures, the adsorption amount of CO₂ (or CH₄ to a lesser extent) in the small pore was higher than that in the larger ones. The preadsorbed water content affects competitive sorption of methane and carbon dioxide onto clays. Our molecular simulations demonstrate that CO₂ has a higher affinity for clays and will therefore displace adsorbed CH₄. The ideal adsorbed solution theory agreed well with the adsorption capacities and selectivities of CO₂/CH₄ mixture. The mobility of CO₂ in the interlayers of clays, at fixed loading of CO₂, is not much affected by CH₄. The presence of adsorbed CO₂ molecules, at fixed amount of CH₄, very much reduced the self-diffusion coefficients of CH₄, and relatively larger decreases in those coefficients are acquired at higher loadings. At reservoir conditions, the adsorption of CO₂ in the dehydrated interlayer is inhibited, followed by the expansion of the interlayer space due to uptake of water and CO₂ as the relative humidity increases. The type of cation does not affect much the mobility of CO₂ in each hydration state in accordance with the fact that CO₂ molecules rarely move into the first hydration sphere of the interlayer cations.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-E / 972

Molecular Simulation of Competitive Adsorption behaviors of CO₂/CH₄ Mixtures on Shale Clay Minerals

Author(s): Xiaofei Hu¹ ; Yuanyuan Tian¹ ; Zhehui Jin²

Co-author(s): Hucheng Deng ¹ ; Changhui Yan ³
Objectives:
CO2 injection, as one of the effective techniques for enhancing recovery of shale gas, has been widely used and proved economically available. In shale, clay minerals play an important role on methane adsorption due to its large volume of micropores. So far, however, a few attentions have been paid on competitive adsorption of CO2/CH4 Mixtures on clay minerals. In this study, we conduct molecular simulations of CO2/CH4 mixtures to provide a better understanding of competitive adsorption behaviors on clay minerals with the grand canonical Monte Carlo (GCMC) simulation.

Methods/Procedures/Process:
We conduct GCMC simulations of CO2/CH4 mixtures adsorption in various clay minerals. Based on the actual conditions of shale gas reservoir, the competitive adsorptions of CO2/CH4 mixtures are investigated at various temperatures of 303.15K, 333.15K, and 363.15K with the pressure range of 0-35Mpa. For comprehensive comparison, the effects caused by pore size, mole fraction of CO2/CH4, and different clay minerals on competitive adsorption are processed. The competitive adsorption behaviors are characterized by selectivity and such key parameter are employed to evaluate the density profiles of CO2 and CH4, the characteristics of CO2 adsorption over CH4, and the timing of CO2 Injection.

Results/Observes/Conclusions:
Due to strong quadrupole moment and higher van der Waals interactions, CO2 possess a stronger affinity for clay minerals than that of methane, which is nonpolar. CH4 has the characteristic of single-layered adsorption, while the CO2 is able to form multi-layers adsorption with higher adsorption amount. Molecular simulations results show that the selectivity of CO2 in competitive adsorption decrease with decreasing of pressure. In addition, the selectivity of CO2 is independent on temperature. Because of negatively charged silicate layers, CO2 adsorption in nanopores of illite and montmorillonite are stronger than that of in kaolinite. As a result, the selectivity of CO2 in kaolinite models is less than that of in illite and montmorillonite models. When pressure is higher than 10Mpa, however, the selectivity of CO2 in three different clay minerals are similar. Due to the more adsorption sites occupied by CO2, the selectivity increases with mole fraction of CO2. By comparison with different pore size adsorption, the selectivity is insensitive to the mole fraction in micropores, while it increases with the increasing of mole fraction of CO2 in mesopores.

Novelty:
This work is a study on CO2/CH4 Mixtures adsorption behaviors on shale clay minerals. The molecular simulations with GCMC are proposed to give an insight in competitive adsorption mechanism, which is expected to provide a more accurate understanding of CO2 injection for enhancing recovery of shale gas.

References:

Acceptance of Terms and Conditions:
Click here to agree
Corresponding Author(s): lzyx361@163.com

Abstract
Understanding the gas occurrence states under real reservoir conditions is the prerequisite to study
the mechanisms of gas flow in shale reservoirs, in which large amounts of nanoscale organic pores
exist. Besides, water is inevitable when considering the gas flow in shales. Thus molecular dynamics
simulations were performed to study the occurrence states of gas-water mixtures near the organic
solid. Results indicate that methane will approach the organic surface spontaneously, accumulate
at the solid-liquid interface and form a dense gas region finally. This process has little relationship
with gas saturation. Potential of mean force (PMF) was calculated to explain the enrichment of
methane. We found that both the wall-gas interaction and the water-gas interaction are beneficial
to the adsorption of methane and the former takes the leading role, while the gas-gas interaction
impedes the adsorption. In addition, the effects of reservoir temperature, pressure, rock wettability,
and carbon dioxide (CO2) on the occurrence states of methane-water mixtures near the solid surface
were studied. The temperature, rock wettability and CO2 influence the occurrence states near the
surface obviously, while the pressure in the simulating range does not. This study also suggests the
potential of thermal exploitation, altering the rock wettability and CO2 injection to enhance shale
gas recovery.

Key words: shale; gas-water mixtures; organic matter; occurrence state; adsorption; potential of
mean force

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-E / 30

Molecular views on surface-driven flows: the case of thermo-osmosis

Li FU¹ ; Samy MERABIA¹ ; Laurent Joly¹

¹ Université Lyon 1 - Institut Lumière Matière

Corresponding Author(s): laurent.joly@univ-lyon1.fr

Surface-driven flows (also called osmotic flows) are generated at interfaces by various thermody-
namic gradients (e.g. electric potential gradient: electro-osmosis, solute concentration gradient:
diffusio-osmosis, temperature gradient: thermos-osmosis). They represent powerful tools to manip-
ulate liquids in micro and nanofluidic systems, and play a key role in living systems, in sustainable
energies, or in water treatment and desalination processes. Osmotic flows arise from the coupling
between hydrodynamics and liquid-wall interactions in the nanometric vicinity of the interface, and
yet standard descriptions are usually based on continuum models and liquid-wall interactions only.
During this talk I will illustrate with recent work on thermo-osmosis how molecular dynamics sim-
ulations can be used to investigate the mechanisms underlying surface-driven flows. In this work,
our main objective was to understand the effect of the wetting properties of the liquid on the solid
surfaces. We have shown the critical role of interfacial hydrodynamics, which can reverse the di-
rection of the flow, and strongly amplify it. In particular, we have predicted giant thermos-osmotic
flows at the water-graphene interface. These theoretical results open many perspectives for the
efficient generation of flows using waste heat, which could be applied for instance to sea water
desalination.

References:

  Lett. 113, 088301.

• A. Barbosa de Lima, L. Joly (2017). Electro-osmosis at surfactant-laden liquid-gas interfaces: be-


Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-H / 561

Moment Equations for Tracer Solute Transport in Composite Media with uncertain dispersivities.

Alberto Guadagnini¹ ; Aronne Dell’Oca¹ ; Monica Riva¹ ; Philippe Ackerer²

¹ D Dipartimento di Ingegneria Civile e Ambientale (DICA), Politecnico di Milano
² E Laboratoire d’Hydrologie et Géochimie de Strasbourg, University of Strasbourg/EOST/ENGEES, CNRS UMR 7417

Corresponding Author(s): alberto.guadagnini@polimi.it

Characterizing dissolved chemical migration in porous media through the Advection Dispersion Equation requires the knowledge of the fluid velocity field and of dispersivity values associated with diverse geomaterials which can make up the internal architecture of the system. Several studies have focused on the assessment of the impact on solute concentration dynamics of an incomplete knowledge of the fluid velocity field, the latter being typically due to uncertainty of hydraulic properties of the hosting media (e.g., permeability). Limited attention has been devoted to analyze the way uncertainty about spatial distribution of dispersivity values can propagate to uncertainty of solute concentration fields. Here, we address this issue by focusing on a simple one-dimensional domain filled with two distinct porous media and subject to a pulse injection of a tracer. We derive and solve numerically the equation governing the expected value and associated variance of solute concentration by considering uncertain dispersivity values and conceptualizing the domain as a random composite medium (where the location of the interface between the two materials can be uncertain). The solutions of such moment equations compare well against corresponding moments evaluated through a numerical Monte Carlo analysis. Our results suggest that in the investigated set-up (i) solute concentration variance exhibits a three peaks behavior, even in the presence of conditioning on a given location of the interface between the two materials and (ii) the actual sequence of the materials traveled by the solute impacts spatial distributions of expected value and variance of concentrations.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-D / 896

Morphological Evolution of Invading Fluids under Homogeneous and Heterogeneous Wetting Conditions

Weiwei Li¹ ; Martin Brinkmann² ; Hagen Scholl¹ ; Ralf Seemann³ ; Pegah Shakeri³

¹ Saarland university/MPIDS
² Saarland University
³ Saarland University/MPIDS
Corresponding Author(s): weiwei.li@physik.uni-saarland.de

Wettability is a major factor that controls the evolution of interfaces during immiscible fluid displacement from a permeable medium. Three dimensional imaging by ultrafast X-ray tomography allows us to investigate the morphology at different wetting conditions and relate it to the prevalent pore-scale process. In this study we focus on the evolution of the fluid interfaces in random piles of spherical beads with a narrow radius distribution. The contact angle of the invading fluid is varied through surface functionalization and by using different combinations of invading and defending fluids. Three methods are proposed to quantify the morphology of the invading interface from the acquired X-ray images. As governed by the contact angle, two qualitatively different classes of displacement pattern are observed in homogeneous bead packs of uniform wettability [1]. The same contact angle for the cross-over between the two distinct displacement regimes is obtained applying three independent methods to quantify the morphology of the invading fluid. Samples consisting of wettable and non-wettable beads indicate that the displacement pattern is the result of a mixture of different local advancing modes of the interface. These modes lead to either capillary fingering or stable front invasion [1]. The influence of wettability is further delineated by varying the ratio between wettable and non-wettable beads in the packing. Our results demonstrate the strong influence of mixed wet conditions on the displacement process, and provide further insights to the factors that control the formation of the macroscopic fluid flow pattern.

Reference:

References:

Parallel 5-D / 86

Multi-Step Segmentation Protocol for Digital Rock Systems

Chaitanya Pradhan\textsuperscript{none}; Majeed Shaik\textsuperscript{none}

Corresponding Author(s): chaitanya.pradhan@shell.com

A key element in digital rock physics is the segmentation of µ-CT scanned grayscale images into their constituent components, i.e. rock and pore. In this work, a multistep approach of segmentation is presented where the high degree of correlation present in neighboring voxels is utilized. The first step in the workflow is a modified fuzzy c-means algorithm which incorporates spatial information in the membership function during the clustering process [1]. This process segments the image into regions corresponding to the rock phase, the pore phase and the unsegmented phase based on the degree of membership. This information is then used as a priori knowledge to complete the segmentation using a method inspired by indicator kriging [2]. This method is advantageous as it reduces spurious blobs and is less sensitive to noise as compared to conventional segmentation algorithms such as Otsu and watershed. These segmented images are then used in simulators to obtain petrophysical properties such as porosity, permeability and capillary pressure curves which are validated against experimental values.

References:

Acceptance of Terms and Conditions:
Click here to agree
Multi-component diffusion in a coupled free-flow porous-medium system

Katharina Heck¹ ; Rainer Helmig ²

¹ University Stuttgart ² University of Stuttgart

Corresponding Author(s): katharina.heck@iws.uni-stuttgart.de

A standard approach to model diffusion in porous media is the assumption of the validity of Fick’s Law. Although widely used, that description can only be employed for binary mixtures or low concentrations of the components as it neglects molecular interactions of the different species. When looking e.g. at gas migration of an organic component in soil where higher concentrations of components can occur, more complex laws need to be employed. In this work we present a multi-phase, multi-component model incorporating the Maxwell-Stefan’s approach to diffusion which takes into account all interactions between the molecules of different species. Therefore it is possible that the diffusion behaviour is very different to the one seen in the standard continuum advection-diffusion description.

We present a coupled free-flow porous-medium model, where the Maxwell-Stefan diffusion approach is employed in both domains. Consistent coupling conditions for coupling the free-flow domain to the porous medium are presented as well.

The model is implemented in the numerical software framework DuMuX and can be used for various applications. The example application presented is a study on evaporation together with gas migration in the porous medium and across the porous-medium free-flow interface. Different concentrations of the gas components and their influence on evaporation rates and gas migration rates across the porous-medium free-flow interface are compared.

References:

Acceptance of Terms and Conditions:

Click here to agree

Invited 1 (Room A) - Takeshi Tsuji / 1111

Multi-phase fluid behaviors with various capillary numbers, viscosity and wettability: Insight into effective and safe CO2 storage

Takeshi Tsuji¹

¹ 1. Department of Earth Resources Engineering, Kyushu University, Fukuoka, Japan 2. International Institute for Carbon-Neutral Energy Research (WPI-i2CNER), Kyushu University, Fukuoka, Japan

Corresponding Author(s):

The behavior of CO2 inside a reservoir (i.e., two-phase flow in CCS, or three-phase flow in CCUS) is influenced by interfacial tension, pore structure, wettability and other reservoir parameters (e.g., pressure gradient), which vary significantly from one reservoir to the next. Therefore, understanding multi-phase flow under various reservoir conditions is crucial to estimating CO2 storage capacity, leakage risk, and storage efficiency. In this study, we calculated two-phase or three-phase fluid displacements in natural digital rocks using lattice Boltzmann (LB) simulation, and characterized the influence of reservoir conditions (e.g., interfacial tension, pressure gradient, and wettability) upon CO2 behavior. By mapping the CO2 saturation on the diagram of capillary number and viscosity ratio of the two fluids, we could identify the suitable environments for effective CO2 storage. We further calculated two-phase and three-phase relative permeability of digital rocks under various conditions. Porous flow simulation also contributes to geophysical monitoring of CO2 behavior in reservoirs. For example, we calculated geophysical properties (e.g., seismic velocity) of the digital
rocks with injected CO2 under various reservoir conditions. Using the relationship between seismic velocity and CO2 saturation parameterized by reservoir conditions, we could quantify in situ CO2 saturation in reservoir from geophysical monitoring data (seismic velocity). In this presentation, we would like to show how porous flow simulations practically contribute to the safe and effective CO2 storage.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-D / 203

Multi-scale 3D pore network characterization of building materials

Author(s): Steven Claes

Co-author(s): Wouter Van De Walle ; Islah Islahuddin ; Hans Janssen

1 KULeuven - Department of Civil Engineering - Building Physics Section

Corresponding Author(s): steven.claes@kuleuven.be

Three-dimensional (3D) analyses of the pore structure of building materials are becoming progressively more important in recent years in order to get more accurate interpretations and simulations of moisture and heat transfer properties. These characteristics are a major determinant for the durability and sustainability of structures as well as for the health and comfort of the building occupants. Building materials are characterized by a large variety in pore radii (e.g., nanometer to millimeter scale) that influence these characteristics. The problem of constructing a pore level model at the representative scale, must be solved by including information from each length scale of this multi-scale system.

Two different imaging techniques are used to visualize the pore structure at different scales. On a micrometer scale computed tomography (CT) has proven to be an excellent and versatile tool to perform these analyses non-destructively. To visualize even smaller pore structures of building materials on the nanoscale, scanning electron microscopy combined with focused ion beam (FIB-SEM) is used. Post processing of the 2 dimensional FIB-SEM images results in a reconstruction of the 3D pore space. Both techniques allow calculating relevant parameters such as pore size, shape and orientation in 3D. Additionally, the pore network is also indirectly characterized by mercury intrusion porosimetry (MIP), resulting in a validation of the results of the direct imaging techniques with a multi scale MIP analysis.

Moreover, building materials are often non-granular in nature, resulting in pore networks comprising of complex pore shapes. Hence, these materials are ideal test cases for pore-shape analysis. We will look at different shape descriptors using the ratios of the longest, intermediate, shortest dimensions and compactness of the pore shapes, based on an approximating ellipsoid, in order to obtain a thorough and objective description of pore shapes as well as their orientation.

Also the study of the Representative Elementary Volume (REV) of these different parameters is necessary to assess the quality of the model. Because the used datasets transient different length scales, the results of the REV analysis will be compared to the observations of Norris et al. (1991) and Nordahl and Ringrose (2008) for geological samples. They both suggested the existence of different REV sizes at different scales which has major implications when determining a relevant upscaling strategy.

References:
References:
Click here to agree

Poster 1 / 213

Multi-scale CO2–Brine Core Flooding Under X-Ray CT In Sandstone From Ordos Basin

Author(s): Yan WANG

Co-author(s): Dustin Crandall ; Liwei Zhang ; Ning WEI ; Xiaochun Li ; Johnathan Moore ; Grant Bromhal

1 State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese
Academy of Sciences
2 Institute of Rock and Soil Mechanics, Chinese Academy of Sciences
3 AECOM, National Energy Technology Laboratory
4 Department of Energy, National Energy Technology Laboratory

Corresponding Author(s): ywang@whrsm.ac.cn

To understand how does the injected CO2 migration could help increase the available storage capacity in geologic formations, this paper reports a series of experiments of core flooding. To examine the effects of CO2migration pathways in geologic formations, our team have developed a core flooding test of displacing water in porous media with CO2. The samples were obtained from the Ordos Basin, all formations being used for carbon capture and storage(CCS) pilot—Shenhua CCS demonstration project, with a capacity of 100,000 tones CO2 per year, which is the first fully process of CCS in saline reservoir in China. All flooding tests in this paper were performed in the industry CT scanner, medical CT scanner and micro CT scanner. Experiments were performed over several weeks by injecting CO2-saturated brine through samples. At the same time the samples were scanned with a computed tomography (CT) scanner at regular intervals (0.5mm) during the course of the experiments. Injection flow rates and temperature of the system were varied for each experiment. For the first test of every sample, the helium gas as the flow constant pressure 100 psi at different flow rates (0.72ml/min, 1.48 ml/min, 2.96 ml/min) was test. Then the brine and CO2 as the flow constant pressure 2000 psi at different flow rates (1.72ml/min, 3.43ml/min, 5.13 ml/min) was test. The constant injection pressure resulted in unstable flow patterns. For the subsequent tests a constant injection rate was set with the Isco pumps and with additional software controls to ensure the pore pressure did not exceed the confining pressure (2500 psi). As long as the injection pressure was less than the confining pressure the flow rate was constant for a constant delta pressure. When the injection pressure increased to a value close to the confining pressure the flow rate was decreased to ensure safe operations. A review of the findings in common among the studied is presented in the final sections of this paper.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-E / 295
Multi-scale granular porous structure generation and its effect on permeability

Moran Wang\textsuperscript{None} ; Tong Liu\textsuperscript{None}

Corresponding Author(s): t-liu15@mails.tsinghua.edu.cn

Multi-scale nature is one of the key features in complexity of rock structures from unconventional resources. Advanced imaging techniques such as high resolution Computed Tomography (CT) and Focused Ion Beam–Scanning Electron Microscopy (FIB-SEM) have shown that these low permeability rocks possess bi-model pores distribution. To characterize the inter-particle and intra-particle pores and their influence on permeability is important for economically imaging unconventional rocks and effectively predicting the rock permeability.

Experiments are powerful in providing direct information and classification of the inter-particle and intra-particle pores, however heterogeneity makes it difficult to distinguish influence of pores at varying scales. To investigate separate influence of inter-particle and intra-particle pores on permeability, numerical generation of multi-scale rock structure and numerical calculation of permeability are necessary.

In this work, a multi-scale porous structure generation method is brought up and the permeability is computed with Lattice Boltzmann Method (LBM). The generation method is based on Random Generation Growth (RGG) method and only particle morphology is considered at present. By assuming that the rock is formed by porous particles, which consist of smaller agglomerated particles, RGG are used under two scales to control the porous particle structure (intra-particles pores) and the entire packing structure (inter-particle pores). Simulation results by LBM are firstly validated with liquid chromatography experiments data. Then individual influence of inter-particle and intra-particle pores is studied in detail. It is shown that intra-particle pores help to improve the structure permeability and with decreasing intra-particle pore size and porosity, the influence of intra-particle pores can be neglected.

References:


Click here to agree

Parallel 5-H / 623

Multi-scale modeling of coupled diffusion-electrochemical reaction for porous micro-electrodes incorporating enzymatic catalysis

Tien Dung Le\textsuperscript{None} ; Didier Lasseux\textsuperscript{1} ; Alexander Kuhn\textsuperscript{2} ; Nicolas Mano\textsuperscript{3} ; Gerard Vignoles\textsuperscript{4}

\textsuperscript{1} I2M Bordeaux
\textsuperscript{2} Institute of molecular science (IMS)
\textsuperscript{3} Centre de recherche Paul Pascal (CRPP)
\textsuperscript{4} Laboratoire des Composites Thermostructuraux (LCTS)
Corresponding Author(s): didier.lassaux@ensam.eu

Porous electrodes with high specific surface area have been efficiently applied to design miniaturized electro-devices such as bio-batteries, bio-captors, etc. Such electrodes may provide much higher electrical current than classical flat electrodes of the same macroscopic size \(^1\). In a previous work \(^4\), a multi-scale model of diffusion and electrochemical reaction in porous electrodes has been developed for a simple oxygen reduction reaction so that oxygen is reduced to hydrogen peroxide by directly consuming electrons at the cathode. In order to improve the efficiency of such devices, redox reactions may be catalyzed by enzymes which are immobilized within a polymer layer in the vicinity of the solid surface \(^2\). In the present work, we develop a multi-scale model of coupled transport and electrochemical reaction in porous electrodes operating in the enzymatic Direct Electron Transfer regime where complex reactions induced by the enzymes together with their mass balance are taken into account.

At the microscopic pore-scale, an electrochemical model for complex redox enzymatic reactions at the solid-fluid interface is developed, considering the oxygen reduction reaction which is catalyzed by the bilirubin oxidase enzyme (BOD) at the cathode. In this scenario, the Butler-Volmer equation is used to relate the potential and reaction rates with the current. This electrochemical model is further coupled with the mass transfer of oxygen governed by Fick’s law and the mass balance of enzymes to form the microscopic coupled model in transient regime. By making use of the volume averaging method \(^3\), the above mentioned microscopic problem is upscaled to obtain a macroscopic model. This model is characterized by a macroscopic coupled diffusion-reaction equation in the porous electrode involving an effective diffusion coefficient that can be computed from the solution of an intrinsic closure problem. Using a model pore geometry, 3D direct numerical simulations of the microscopic model are carried out and compared to 1D numerical simulations of the macro-model. Excellent agreement between the oxygen concentration profiles within the electrodes obtained from the two models is observed while a speed-up of about 21600 is achieved with the 1D macro-model illustrating the capability of the multi-scale approach. Such a model is capable of providing an accurate estimation of the electrical current density with respect to the pore-space architecture providing a useful tool for electrode microstructural optimization. A successful comparison between the model and experiments is also reported.

Keywords: Porous electrode, Diffusion, Reaction, Volume averaging, Enzyme.

References:


Click here to agree

Poster 2 / 663

Multi-scale pore imaging techniques to characterise heterogeneity effects on flow and transport in complex carbonate rock

Author(s): Saurabh Shah

Co-author(s): Edo Boek \(^2\); Farrel Gray \(^1\), John Crawshaw \(^1\)

\(^1\) Imperial College London
\(^2\) Queen Mary University of London
**Corresponding Author(s):** saurabh.shah10@imperial.ac.uk

Digital rock analysis and pore scale studies have become an essential tool in the oil and gas industry to understand and predict the petrophysical and multiphase flow properties for the assessment and exploitation of hydrocarbon reserves. The fundamental problem in pore-scale imaging and modelling is how to represent and model the different range of scales encountered in porous media, from the pore scale to macroscopic petrophysical and multiphase flow properties. Carbonate rocks are characteristically heterogeneous. It remains very challenging to describe flow and transport in carbonates because of complex pore structure and connectivity, comprising length scales from tens of nanometers to several centimeters [2].

In this study we investigate the effect of pore structure and connectivity on the flow properties for a Keton carbonate by integrating different 3D imaging techniques. These include 3D micro-CT imaging at four different (4 μm, 6 μm, 8 μm and 10 μm) voxel resolutions; FIB imaging with voxel resolution of 12 nm; and 3D high resolution wide field of view CLSM images [3,4]. Pore Network and Lattice-Boltzmann [5] simulation methods are then used to predict the single and multi-phase flow properties in comparison with experimental data. We also shed new light on the existence and size of the Representative Element of Volume (REV) for 8 different types of porous material specifically rocks ranging from headpacks, sandpacks to sandstone to carbonate rock capturing the different scales of heterogeneity from the pore-scale imaging.

References:


Click here to agree

**Parallel 3-A / 572**

**Multiphase Flow and Underpressured Shale at the Bruce nuclear site, Ontario, Canada**

**Author(s):** Michael Plampin

**Co-author(s):** Christopher Neuzil

1 U.S. Geological Survey

**Corresponding Author(s):** mplamp@usgs.gov

A deep geologic repository (DGR) for low- and intermediate-level radioactive waste has been proposed at the Bruce nuclear complex on the eastern flank of the Michigan Basin in southeastern Ontario, Canada. The proposed location for the repository is at a depth of ~680 m, in the middle of a ~450 m-thick sequence of Ordovician-aged shale and limestone with extremely low porosity and permeability, which makes fluid flow and mass transport processes very slow. Significant underpressure exists in these rocks, and questions have been raised about whether gas phase methane is present and how it relates to the generation and persistence of the underpressure here, as well as those in numerous other shale- and gas-rich sedimentary basins around the world. Multiphase flow simulations have suggested that water can become underpressured in the presence of gas phase due to transient glacial loading cycles, and a previous modeling study of the Bruce site, in which the presence of gas phase was approximated using ad hoc adjustments to single-phase flow parameters, showed that underpressures can persist for geologically significant periods of time. However, while multiphase
interaction and migration processes have been studied extensively for conventional petroleum and environmental engineering applications, they are relatively poorly understood in low-permeability argillaceous rocks such as those at the DGR. The goals of this study are to: (1) determine which rock and fluid parameters are most critical for understanding the multiphase flow processes that may have occurred in the low-permeability formations at the Bruce site through geologic time, (2) assess uncertainty in our understanding of those parameters, and (3) investigate, using the multiphase flow simulator TOUGH2-EOS7C, whether the presence of gas phase methane could have generated or contributed to the underpressure. Results suggest that the presence of gas phase methane does not by itself fully explain the underpressure.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-D / 557

Multiphase flow in shale fracture networks applicable to hydrocarbon recovery processes: huff-and-puff, water displacement, and chemical additives using microfluidic experiments

Author(s): Phong Nguyen

Co-author(s): Bill Carey ¹; Qinjun Kang ²; Hari Viswanathan ²; Mark L. Porter ³

¹ Los Alamos National Lab
² Los Alamos National Laboratory
³ Bureau of Reclamation

Corresponding Author(s): pnguyen@lanl.gov

Current hydrocarbon recovery methods in hydraulically fractured shale have low recovery efficiency of about 10%. The objective of this work is to investigate several enhanced recovery methods to improve the production rates in shale. We examine the effectiveness of nitrogen and supercritical carbon dioxide in huff-and-puff methods for enhanced oil recovery to re-energize the reservoirs and improve recovery rates. In addition, we also present studies of water displacement in fracture networks as a baseline comparison as well as the effects of chemical additives (surfactants and friction reducer). We use direct visualization in microfluidic systems to reveal the mechanisms and to quantify the recovery rates of oil from fracture networks. We compared the effectiveness of water, nitrogen and supercritical carbon dioxide at reservoir conditions in a process mimicking huff-and-puff methods in both dead-end and connected fracture systems. Water and chemical additives were also used to study multiphase displacement mechanisms. The chips are made of glass and shale and placed in a confining pressure system pressurized to 10 MPa, 50 oC. The system was allowed to equilibrate, and then depressurized to determine oil recovery. Fluorescent microscope images were continuously taken to visualize and calculate residual oil saturation as a function of pressure draw-down. For huff-and-puff experiments, during depressurization from 10 MPa, gas exsolve from the oil liquid phase, including bubble nucleation and coalescence, appeared to be the main energy driver for mobilizing the oil from the fracture networks. Injection of supercritical CO2 had the highest recovery rate and removed most of the initial oil in place; N2 removes about 30% of oil; and injection of water had a negligible recovery rate. The connected fracture network allowed for more gas to dissolve into the oil and had better recovery rates than in the dead-end fracture network. For water displacement tests, we investigate the effects of flow rate and chemical additives in lowering the oil/water interfacial tension, and rock surface wettability on hydrocarbon recovery rates. The mechanisms of oil mobilization, oil saturation, and water displacement patterns, and effectiveness of chemical additives observed in this study can be used to improve the recovery rates in shale through enhanced hydrocarbon recovery methods.

References:

Acceptance of Terms and Conditions:
Poster 2 / 478

Multiphase micro-continuum models: an hybrid-scale approach

Cyprien Soulaine¹ ; Sophie Roman² ; Hamdi Tchelepi³

¹ Stanford University
² Institut des Sciences de la Terre d’Orléans

Corresponding Author(s): cyprien.soulaine@gmail.com

Advances in imaging technologies and high-performance computing are making it possible to perform Direct Numerical Simulation (DNS) of flow processes at the pore scale; nevertheless, the restrictions on the physical size of the sample (porous rock) that can be fully resolved using Navier-Stokes-based DNS are quite severe. For samples on the order of a cm³, the complexity of the spatial heterogeneity of the pore space precludes Navier-Stokes-based DNS. Even for smaller sizes, some microstructures are below the instrument resolution and are not resolved in the image. To deal with this challenge of having a wide range of length scales—even for ‘small’ systems, we describe a micro-continuum formalism, based on the Darcy-Brinkman-Stokes (DBS) equation where flow and transport phenomena are governed by Navier-Stokes equations in the resolved regions (voxels containing fluids only) and by Darcy in the unresolved (solid-fluid aggregates) regions [1]. This hybrid-scale modeling framework has been used successfully to compute the flow in a digital sandstone imaged with X-ray microtomography including sub-voxel porosity [2]. The micro-continuum DBS approach has also been used to simulate dissolution phenomena at the pore-scale under single-phase conditions [3].

In this work, the micro-continuum formulation is extended to multiphase flow where two-immiscible fluids share the pore-space involving surface tension force and moving contact lines at the mineral surfaces. The multiphase micro-continuum model is used to investigate multiphase system with reactive transport and is compared with microfluidic experiments.

References:

Click here to agree

Parallel 3-G / 409

Multiresolution Coupled Compositional Vertical Equilibrium Model for Fast Flexible Simulation of CO2 Storage

Olav Møynæër¹ ; Halvor Møll Nilsen²
CO₂ capture and storage is an important technology for mitigating climate change. Design of efficient strategies for safe, long-term storage requires the capability to efficiently simulate processes taking place on very different temporal and spatial scales. The physical laws describing CO₂ storage are the same as for hydrocarbon recovery, but the characteristic spatial and temporal scales are quite different. Petroleum reservoirs seldom extend more than tens of kilometers and have operational horizons spanning decades. Injected CO₂ needs to be safely contained for hundreds or thousands of years, during which it can migrate hundreds or thousands of kilometers. Because of the vast scales involved, conventional 3D reservoir simulation quickly becomes computationally unfeasible. Large density difference between injected CO₂ and resident brine means that vertical segregation will take place relatively quickly, and depth-integrated models assuming vertical equilibrium (VE) often represents a better strategy to simulate long-term migration of CO₂ in large-scale aquifer systems. VE models have primarily been formulated for relatively simple rock formations and have not been coupled to 3D simulation in a uniform way. In particular, known VE simulations have not been applied to models of realistic geology in which many flow compartments may exist in-between impermeable layers. In this work, we generalize the concept of VE models, formulated in terms of well-proven finite-volume reservoir simulation technology, to complex aquifer systems with multiple layers and regions. The result is a hybrid discretization strategy which couples different governing equations in different regions based on the correct local discretization of gravity and flow terms.

We also introduce novel formulations for multi-layered VE models by use of both direct spill and diffuse leakage between individual layers. This new layered 3D model is then coupled to a state-of-the-art, 3D equation-of-state compositional model. The formulation of the full model is simple and exploits the fact that both models can be written in terms of generalized multiphase flow equations with particular choices of the relative permeabilities and capillary pressure functions. The resulting simulation framework is very versatile and can be used to simulate CO₂ storage for (almost) any combination of 3D and VE-descriptions, thereby enabling the governing equations to be tailored to the local structure. We demonstrate the simplicity of the model formulation by extending the standard flow-solvers from the open-source Matlab Reservoir Simulation Toolbox (MRST), allowing immediate access to upscaling tools, complex well modeling, and visualization features. We demonstrate this capability on both conceptual and industry-grade models from a proposed storage formation in the North Sea. While the examples are taken specifically from CO₂ storage applications, the framework itself is general and can be applied to many problems in which parts of the domain is dominated by gravity segregation. Such applications include gas storage and hydrocarbon recovery from gas reservoirs with local layering structure.

References:
https://arxiv.org/abs/1710.08735 Acceptance of Terms and Conditions: Click here to agree

Parallel 4-G / 280

Multiresolution Operator Decomposition for Flow Simulation in Fractured Porous Media

Author(s): Qinfu Zhang¹
Co-author(s): Houman Owhadi ²; Jun Yao ¹; Florian Schafer ²; Zhaoying Huang ¹; Yang Li ¹

¹ China University of Petroleum (East China)
² California Institute of Technology

Corresponding Author(s): zhangqingfuupc@gmail.com
Fractures should be simulated accurately given their significant effects on whole flow patterns in porous media. But such high-resolution simulation imposes severe computational challenges to numerical methods in the applications. Therefore, the demand for accurate and efficient technique is widely increasing. A near-linear complexity multiresolution decomposition is proposed for solving flow problems in fractured porous media. In this work, discrete fracture model (DFM) is used to describe fractures, in which the fractures are explicitly represented as (n-1) dimensional element. The solution space is decomposed into several subspaces and we then compute the corresponding solutions of DFM in each subspace. The pressure distribution of fractured porous media is obtained by combing the DFM solutions of all subspaces. Numerical results are presented to demonstrate the accuracy and efficiency of the proposed multigrid method. The comparisons with standard method show that the proposed multigrid method is a promising method for flow simulation in fractured porous media.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-H / 540

Multiscale Calculation of Two-phase Flow in Digital Core Analysis

Author(s): Xiaobo Nie

Co-author(s): Jonas Toelke

1 Ingrain, A Halliburton Service

Corresponding Author(s): xiaobo@ingrainrocks.com

Digital core analysis has become an additional tool to physical experimental analysis for multiphase flow experiments. Digital core analysis is fast and can give more insight into the details inside a rock. In digital core analysis different imaging technologies with different resolutions are employed to identify pores and textures scaled from millimeters to nanometers in a heterogeneous rock, such as a carbonate rock. In each resolution the field of view of 3D image volume is up to a few thousand pixel in one direction. Utilizing a highly efficient pore scale simulator and a powerful computer, the size of 3D rock volume that can be practically handled in a multiphase flow simulation is about one thousand pixels in each direction. To compute the multiphase flow properties in a heterogeneous rock with pores scaled from millimeters to nanometers several image resolutions have to be combined. One approach is to compute multiphase flow properties in different scales independently and then upscale them to the whole rock sample. The dynamic flow exchanges in different scales are ignored. Especially the flow path and the wettability changes provided by under-resolved finer scales are ignored. It is also hard to handle the effects of overlapped pores in two images of neighboring scales in the same region in the upscaling.

We developed a scale-coupled multiscale model to calculate two-phase flow distributions for certain capillary pressure (Pc) in the porous plate experiment. The two-phase distributions then can be used to calculate the relative permeability (Kr) and the saturation factor (n) for capillary dominated flow. In the multiscale model, a rock sample in a certain scale is geometrically represented by pores, solids and Darcy regions that have under-resolved pores. Two phase flow in the resolved pore space is directly simulated using a lattice-Boltzmann model (LBM). The two phase flow properties in a Darcy region are given by a prescribed map function. The map function can be obtained in a finer scale simulation or theoretically modeling. The map function gives the two-phase flow properties in a Darcy region based on the flow phases and pressure distributions surrounding the Darcy region. In the meantime the boundary conditions on surface of a Darcy region of LBM simulation in resolved pores depend on two phase properties in the Darcy region. The flow distributions in pore and Darcy regions, and the boundary conditions for different scales dynamically change with applied capillary pressure. The scale coupled calculation starts from the finest scale. The calculated two phase flow properties, such as Pc, Kr and n, in a finer scale serves as map functions of Darcy regions in the coarser scale calculation. The calculation ends in the coarsest scale, usually the plug or core scale. The scale coupled multiscale model of two-phase flow has been tested in different heterogeneous rock samples and two-phase flow properties in different scale levels will be reported.
Parallel 10-G / 558

Multiscale Computation of Pore-Scale Fluid Dynamics

Yashar Mehnani1; Hamdi Tchelepi1

1 Stanford University

Corresponding Author(s): yashar.mehnani@gmail.com

Understanding the dynamics of fluid flow and transport in porous media is important in several subsurface applications including geologic CO2 storage, hydrocarbon recovery, geothermal energy, and groundwater hydrology. In order to control and optimize said dynamics, it is imperative that these processes be considered at the pore (or micro) scale. Pore-scale models provide a useful means of approaching such problems. However, current direct numerical simulation (DNS) methods can be prohibitively expensive, even though they produce the highest fidelity predictions. On the other hand, certain surrogate models (e.g., pore-network models) are considerably less expensive and can be used to approximate the fluid flow physics in porous media. However, current surrogate models often lack the ability to control/shrink their prediction errors. In other words, the concept of “convergence to a solution” is absent. In this work, we present a new computational framework for simulating fluid flow dynamics at the pore scale. We demonstrate that through a combination of multiscale, multiresolution, and domain decomposition concepts the Navier-Stokes equations can be solved very efficiently on porous materials with structures of arbitrary complexity. Moreover, the framework provides the ability to converge, in a step-by-step fashion, to the full DNS solution through successive iterations. This renders the approach flexible for a variety of applications in/outside geosciences, which pose different tolerances for error.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-H / 662

Multiscale Data Assimilation of Spatially Distributed Information

Author(s): Rafael Moraes1

Co-author(s): Hadi Hajibeygi 1; Jan Dirk Jansen 1

1 TU Delft

Corresponding Author(s): r.moraes@tudelft.nl

In data assimilation problems, various types of data are naturally linked to different spatial scales (e.g. seismic and electromagnetic data), and these scales are usually not coincident to the subsurface simulation model scale. Alternatives like down/upscaling of the data and/or the simulation model can be used, but with potential loss of important information. To address this issue, a novel Multiscale (MS) data assimilation method is introduced. The overall idea of the method is to keep uncertain parameters and observed data at their original representation scale, avoiding down/upscaling of any quantity. The method relies on a recently developed mathematical framework to compute Adjoint gradient via a MS strategy [2, 3]. The fine-scale uncertain parameters are directly updated and the
MS grid [4, 5] is constructed in a resolution that meets the observed data resolution. The advantages of the technique are demonstrated in the assimilation of data represented in a coarser scale than the simulation model. The misfit objective function is constructed to keep the MS nature of the problem. The regularization term is represented at the simulation model (fine) scale, whereas the data misfit term is represented at the observed data (coarse) scale. The performance of the method is demonstrated in synthetic models and compared to down/upscaling strategies. The numerical experiments show that the MS strategy provides advantages on the computational side – expensive operations are only performed at the coarse scale; on the accuracy – the matched uncertain parameter distribution is closer to the “truth” model; and in the optimization performance – faster convergence behavior and smaller OF value are obtained. As conclusion, the newly developed method is capable of providing superior results when compared to strategies that rely on the downscaling of the observed data, addressing the scale dissimilarity via a robust, consistent MS strategy.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-A / 26

Multiscale Hybrid Discontinuous Galerkin method applied to homogenization problems.

Manuela Bastidas1; Sorin Pop1

1 Hasselt University

Corresponding Author(s): manuela.bastidas@uhasselt.be

In this presentation we present a numerical method for simulating fluid flow in highly anisotropic and heterogeneous porous media. To understand the behavior of the fluids at the scale of applications (the macro scale), the flow at the scale of pores (the micro scale) needs to be taken into account. In this case, standard numerical methods will either fail or become inefficient due to the complexity of the flow domain.

We present a numerical scheme based on Hybridized Discontinuous Galerkin (HDG) formulation to compute the upscaled behavior of fluids in a porous media, which can include reactive transport and free boundaries in the micro scale. The scheme is a multiscale HDG method that applies generally to elliptic or parabolic problems in complex domains, and involving strongly oscillating characteristics. This method is based on the classical homogenization technique and the results are presented in terms of the convergence of the error in the micro and macro scale.

Finally, we discuss different combinations of the approximation polynomial spaces on both scales and show the advantages of each one compared with the multiscale mixed finite element approach.

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 11-F / 838

Multiscale characterisation of and flow simulation in the nanoporous structure of shale matrix: challenges and solutions

Yudong Yuan\(^1\); Yuzhu Wang\(^1\); Sheik Rahman\(^1\)

\(^1\) UNSW, Sydney

Corresponding Author(s): yydcug@163.com

Shale is a fine-grained sedimentary rock. Flow simulation in shale is challenging due to its multiscale porous structure (consisting of nano- to micropores and fractures) and multi-physics gas flow mechanism (including continuum flow, slip flow, transition flow, Knudsen diffusion and surface diffusion) in these pores. The available studies have provided preliminary understandings on the porous structure of shale and flow processes within that; however, the reliability of these models depends on the representativeness of the structures and accuracy of flow models, which are hindered by the difficulties including, but not restricted: (1) FIB-SEM can provide high-resolution images but the field of view is much smaller than the scale of measurable samples in lab; (2) traditional definition of mean free path of gas molecules may be inaccurate when gas adsorption occurs in the nanopores; (3) discrepancies exist regarding the equations describing flow in the single capillary, which is the basis of flow simulation in porous structure; (4) gas-water flow pattern in nanopores is yet well understood; (5) contribution of nano-scale matrix permeability to the productivity is controversial. In this study, the challenges of these issues are analysed with the aids of thorough review of literature and potential solutions, including multiscale image reconstruction, molecular dynamics simulation and pore network modelling, are proposed. This study may give insights into the multiscale flow simulation in the nanoscale porous media and point out the future direction for researchers.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-C / 625

Multiscale characterization of carbonate rock deformation induced by coupled chemo-mechanical processes during core flooding

Hongkyu Yoon\(^1\); Thomas Dewers\(^1\); Jan Ludvig Vinningland\(^2\)

\(^1\) Sandia National Laboratories
\(^2\) International Research Institute of Stavanger

Corresponding Author(s): hyoon@sandia.gov

Coupling of geochemical reactions with hydrological and mechanical processes in nano-porous carbonate rocks can lead to complex behaviors involving the change of pore topology (e.g., precipitation, dissolution, compaction) and mineralogy. Fluid-rock interactions also change hydrological, mechanical, and geophysical properties (e.g., permeability, rock strength, elastic, acoustic velocity) across spatial and temporal scales. Here we analyzed a Liège chalk sample that have been flooded with MgCl2 in a triaxial cell for 516 days, which was compared to unflooded sample. To identify the impact of chemo-mechanical coupling on the change of mineralogy, pore-structure, and mechanical properties, various multiscale imaging techniques were applied and nano-indentation testing was performed. Multiscale imaging includes dual focused ion beam-scanning electron microscopy (FIB-SEM), micro computed tomography (micro-CT), 2D and 3D energy dispersive spectroscopy (EDS), backscattered electron microscopy (BSE), and MAPS mineralogy. First, we obtained 2D mineralogical mapping and pore structures over a large sample area (~ 0.4cm x 2cm) using EDS and BSE, respectively, to determine the locations of FIB-SEM analysis. The mineralogical mapping reveals the interface of reaction front and the textural fabrics revealed by FIB-SEM images (i.e., 1000 image stacks) at 10 nm resolution and elemental mapping by 3D FIB-EDS at 10 nm resolution show
alteration patterns due to dissolution, precipitation, and compaction compared to unaltered sample with clear grain boundary. FIB-SEM-EDS images of the altered sample at multiple locations show distinct pore features including discrete micro-cracks in the chemically unaltered zone, sharp precipitation boundaries in the chemically altered zone, and smooth and relatively large pore space in the boundary zone of chemical reaction. Nano-indentation testing at multiple scales is performed to evaluate the impact of the change of pore structure and mineralogy on the mechanical properties. Lattice Boltzmann simulations and nano-indentation simulations are used to evaluate the change of permeability and mechanical properties at several different scales. Overall, these results clearly demonstrate that it is very critical to characterize the change of multiscale pore structure associated with chemical reactions and mechanical deformation. Multiscale and multiphysics analysis of coupled processes in nanoporous media with broad compositional range and physical and chemical heterogeneity will enhance a fundamental understanding of poromechanical and flow responses of the materials.

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-NA0003525.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-H / 839

Multiscale model reduction for coupled problems in fractured porous media

Eric Chung\footnote{The Chinese University of Hong Kong} ; Yalchin Efendiev\footnote{Texas A&M University} ; Wing Tat Leung\footnote{Chinese University of Hong Kong} ; Maria Vasilyeva\footnote{Chinese University of Hong Kong} ; Yating Wang\footnote{Chinese University of Hong Kong}

In this work, we consider multi-physics problems (flow, transport, and mechanics) in fractured porous media and present upscaling and multiscale methods for construction of a coarse-grid model. We propose a rigorous and accurate multiscale solver and upscaling framework based on some recently developed multiscale methods. Our proposed method consists of identifying multicontinuum parameters via appropriate local solutions in oversampled regions. The method involves two basic steps: (1) the construction of multiscale basic functions that take into account small scale heterogeneities in the local domains and (2) the macroscopic equations for the coarse-scale model. In contrast to the available techniques, this method can give rigorous upper bounds for the errors. This method also more general technology that takes into account the different scale processes. We present numerical results for a transport and flow problems, poroelasticity problems and problems with dual-continuum background models. Our numerical results show that the proposed approach can provide good accuracy for problems in fractured porous media.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 1106

Multiscale model reduction of artificial ground freezing
Sergei Stepanov¹ ; Maria Vasilyeva²; Denis Spridonov²

¹ North-Eastern Federal University in Yakutsk
² Multiscale model reduction Laboratory, North-Eastern Federal University;

Corresponding Author(s): cepe2a@inbox.ru

Research in geotechnical applications of artificial ground freezing is important task in maintaining the stability of engineering structures in permafrost. Safe design require a correct prediction of the coupled thermo-mechanical behavior of soils. Mathematical model of process of thermal stabilization (artificial freezing) on the classical Stefan model is built.

A feature of the modeling of this problems under consideration is the clearly expressed geometric diversity of the objects being modeled: the small dimensions of the freezing devises and the large dimensions of the modeling domain. Thus, this problems computation may be very expensive. In this regard, to improve the efficiency of calculations, the need arises to develop new computational algorithms. A coarse-scale solver based on Generalized Multiscale Finite Element Method are constructed. The main idea of which method is to construct a small dimensional local solution space that can be used to efficient solution on coarse grid.

We present numerical results of numerical simulation problem in perforated domains in two-dimensional and three-dimensional formulations are presented.

References


References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-B / 969

Multiscale sensitivity analysis of nanoporous materials

Kimoon Um¹ ; Markos Katsoulakis² ; Daniel M. Tartakovsky³ ; Eric Hall⁴

¹ University of California, San Diego
² University of Massachusetts, Amherst
³ Stanford University
⁴ University of Massachusetts Amherst

Corresponding Author(s): hall@math.umass.edu

Ubiquitous uncertainty about pore geometry inevitably undermines the veracity of pore- and multi-scale simulations of transport phenomena in porous media. It raises two fundamental issues: sensitivity of effective material properties to pore-scale parameters and statistical parameterization of Darcy-scale models that accounts for pore-scale uncertainty. Homogenization-based maps of pore-scale parameters onto their Darcy-scale counterparts facilitate both sensitivity analysis (SA) and uncertainty quantification. We treat uncertain geometric characteristics of a hierarchical porous medium as random variables to conduct global SA and to derive probabilistic descriptors of effective diffusion coefficients and effective sorption rate. Our analysis is formulated in terms of solute
transport diffusing through a fluid-filled pore space, while sorbing to the solid matrix. Yet it is sufficiently general to be applied to other multiscale porous media phenomena that are amenable to homogenization.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-E / 761

N2, CO2, and Ar adsorption to characterize micro- and mesopores of shales

Nerine Joewondo\(^1\); Manika Prasad\(^1\)

\(^1\) Colorado School of Mines

Corresponding Author(s): njoewond@mines.edu

The storage and flow mechanisms in shales depend largely on their microstructure. We use two parameters to characterize microstructures, namely specific surface area (SSA) and pore-size distribution (PSD). We use N\(_2\) adsorption at 77K to quantify SSA and PSD of nanopores. There are two limitations of the N\(_2\) adsorption method due to (1) uncertainties in molecular area due to the quadrupole moment of N\(_2\) molecules result in 20% uncertainty in calculated BET SSA, and (2) kinetic restriction of N\(_2\) molecules prevent it to access narrow pores (\(< 0.7\) nm). To circumvent these limitations, we also used other adsorptives, such as CO\(_2\) and Ar, for the measurements.

We present results from adsorption measurements of CO\(_2\) at 273 K and Ar at 77 K on shales and compare them to N\(_2\) adsorption at 77 K. Adsorption measurements with CO\(_2\) at 273 K allows for detailed characterization of ultramicropores (\(< 0.7\) nm), which are inaccessible to N\(_2\) molecules. Our results from CO\(_2\) adsorption reveal significantly larger micropore SSA in comparison to N\(_2\) probed SSA. Ar molecules do not have quadrupole moment and resolve the uncertainties of molecular area for BET calculation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-E / 52

NON-ISOTHERMAL TRANSPORT OF IMMISCIBLE FLUIDS AT LOW CAPILLARY NUMBERS: SURFACE AND LINE CONTRIBUTIONS TO THE DRIVING FORCE

Author(s): Signe Kjelstrup\(^1\)

Co-author(s): Dick Bedeaux \(^1\); Alex Hansen \(^2\); Bjørn Hafskjold \(^1\); Olav Galteland \(^1\)

\(^1\) Norwegian University of Science and Technology, NTNU, Trondheim

\(^2\) NTNU

Corresponding Author(s): signe.kjelstrup@ntnu.no
We derive the entropy production for transport of heat and two immiscible fluids in an inelastic porous material. The representative volume element (REV) is described by its mass, energy and entropy, and a Gibbs equation from which we define the temperature, pressure and chemical potentials (T, p, \(\mu\)) of the REV.

The constitutive equations that follow from the entropy production of the REV can be written for a continuous path in state space. There are three independent driving forces with conjugate fluxes, one for transport of heat and two for transport of two immiscible fluids. The forces contain contributions from surface and line energies, contributions that are important at low capillary numbers.

We show how the equations can be used to predict a Soret effect in the porous material or to compute thermal osmosis. They provide an explanation for observations known since long, that there are deviations from Darcy’s law at low capillary numbers (1-4), also for single phase flow. This has been observed for transport in clay, soil even through glass beads. We find how the volume flow arises, not only from changes in pressure, but also from changes in porosity or saturation of one of the fluids, in temperature or in chemical potentials. We discuss how the relations can be tested by non-equilibrium molecular dynamics simulations or experiments, and present a first test.


References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 11-D / 874

Nano-particles Transport in Complex 2.5D Low Resolution Polymer Rock Based Micro-models

Jagannath Upadhyay\(^1\) ; Daniel Park\(^1\) ; Karsten Thompson\(^2\); Dimitris Nikitopoulos\(^2\)

\(^1\) Louisiana State University
\(^2\) Louisiana State University, Mechanical and Industrial Engineering Department

Corresponding Author(s): jupadh1@lsu.edu

Micro-models are microfluidic devices used to study the transport of fluids in porous media domains. Porous media relevant to subsurface engineering and reservoir applications are 3D in nature. In order to observe and measure the transport and behavior of nano-particles through such media, it is necessary to preserve the 3D characteristics of the relevant geometry and flow while facilitating observation. These requirements are met through the design of 2.5D micro-models which incorporate micro-channel networks with 3D wall structure albeit with one flat wall for observation. Our group has designed such 2.5D micro-models matching fourteen morphological and flow parameters to those of fully 3D actual reservoir rock samples (Boise sand-stone) at a resolutions of 10 microns (depth) and 25 microns (on the plane). This paper presents a novel method of measuring the geometry, 3D particle velocity, particle concentration and particle deposition measurements for flows in such 2.5D micro-models.
A Confocal Micro-Particle Image Velocimetry (CµPIV) technique along with associated post-processing algorithms is presented for obtaining three dimensional distributions of nano-particle velocity, concentrations at selected locations of the micro-model. Instantaneous particle deposition on the inner surfaces at selected regions of the micromodel is also presented. In addition, an in-situ, non-destructive method for measuring the geometry of the micro-model, including its depth, is described and demonstrated. The flow experiments used 860 nm fluorescence labeled polystyrene particles and the data were acquired using confocal laser scanning microscopy. Regular fluorescence microscopy was used for the in-situ geometry measurement along with the use of Rhodamine dye and a depth-to-fluorescence-intensity calibration, which is linear. Monochromatic excitation at a wavelength of 544 nm (green) produced by a HeNe continuous wave laser was used to excite the fluorescence-labeled nano-particles emitting at 612 nm (red). Confocal images were captured by a highly sensitive fluorescence detector photomultiplier tube. Results of detailed three dimensional velocity, particle concentration and instantaneous particle deposition from experiments conducted at flow rates of 100 nL/min are presented and discussed.

The three dimensional geometry reconstructed from fluorescence data was used as the computational domain to conduct numerical simulations of the flow in the as-tested micro-model for comparisons to experimental results. The flow simulation results is used to qualitatively compare with velocity distributions of the flowing particles. The comparison is qualitative because the particle sizes used in these experiments may not accurately follow the flow itself given the geometry of the micro-models. These larger particles were used for proof of concept purposes, but the techniques and algorithms used in this work will permit future use of particles as small as 50 nm.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 215

Nanoparticle heterogeneous adsorption in porous media

Gaëtan Gerber¹ ; Dave WEITZ² ; Philippe Coussot³

¹ ENPC - Harvard SEAS
² Harvard University
³ Univ. Paris-Est

Corresponding Author(s): gaetan.gerber@ifisttar.fr

Colloidal particles released by various chemical and industrial processes penetrate soils and groundwater, and transport themselves other contaminants like heavy metals or PCBs. Thus, an accurate description of the transport and retention of these particles is required to prevent and manage environmental contamination, like the pollution of drinking water supplies. Literature stands that colloid sorption (also referred to as attachment) is the main process controlling transport in the case of strong particle-medium interactions and absence of straining events. Sorption mechanisms have been widely studied using micromodels (2D systems or pore scale studies [2,3]) or indirect observation (Breakthrough curves [6]), completed by simulations to account for the complexity of real media like soils [7]. We propose here to tackle the usually neglected impact of the system’s heterogeneity, in direct 3D visualizations at local and global scales.

Glass beads at random close packing are chosen as a model porous medium for their large pore throat size distribution (down to 0 at contact points). We inject in the system suspensions of iron nanoparticles (NPs), with a strong attraction interaction with the medium, which leads to heterogeneous adsorption and coverage of the beads. Coverage is followed by confocal imaging in time and at multiple scales; from local singular geometries (pore scale, tens of µm) to global average behaviours (sample’s scale, cm).

We show that for a given NPs-medium affinity, the dynamics of adsorption strongly depend on the accessibility of the surface, in accordance with the flow streamlines. We identify configurations
(regions of highest confinement, i.e. contact points between beads) where the adsorption is fully diffusion limited. At early stages of adsorption, these regions can account for up to 10% of the surface of the medium and therefore impact the supposedly known dynamics at global scale.

To go further, we link local observations and global description of the dynamics to discuss the impact of the pore size heterogeneity, at various flow rates (Darcy velocities in the range 0.05 to 9 mm/s). We show the impact of the flow on the heterogeneity of the deposition of the NPs through 1D coverage profiles over time and over the whole sample. Finally, we propose a simple model describing the full beads coverage dynamics over space and time. We can define and decouple a geometric (characteristic deposition length) and a kinetic (characteristic exploration time) components for a complete understanding of the adsorption mechanisms.

Figure – (Left) Confocal sections of a glass beads pack partially saturated with NPs. From a clean medium, progressive adsorption of nanoparticles at the beads surface is followed by fluorescence. Local and global studies (Right) highlight variations of the dynamics due to the heterogeneity of the medium: confined areas (blue) are covered later and slower than areas directly accessible to the flow.

References:
Click here to agree

Poster 2 / 901

Nanoparticle heterogeneous adsorption in porous media
Gaëtan Gerber¹ ; Dave WEITZ² ; Philippe Coussot³

¹ ENPC - Harvard SEAS
² Harvard University
³ Univ. Paris-Est

Corresponding Author(s): gaetan.gerber@ifsttar.fr

Colloidal particles released by various chemical and industrial processes penetrate soils and groundwater, and transport themselves other contaminants like heavy metals or PCBs. Thus, an accurate description of the transport and retention of these particles is required to prevent and manage environmental contamination, like the pollution of drinking water supplies. Literature stands that colloid sorption (also referred to as attachment) is the main process controlling transport in the case of strong particle-medium interactions and absence of straining events. Sorption mechanisms have been widely studied using micromodels (2D systems or pore scale studies [2,3]) or indirect observation (Breakthrough curves [6]), completed by simulations to account for the complexity of real media like soils [7]. We propose here to tackle the usually neglected impact of the system’s heterogeneity, in direct 3D visualizations at local and global scales.
Glass beads at random close packing are chosen as a model porous medium for their large pore throat size distribution (down to 0 at contact points). We inject in the system suspensions of iron nanoparticles (NPs), with a strong attraction interaction with the medium, which leads to heterogeneous adsorption and coverage of the beads. Coverage is followed by confocal imaging in time and at multiple scales; from local singular geometries (pore scale, tens of μm) to global average behaviours (sample’s scale, cm).

We show that for a given NPs-medium affinity, the dynamics of adsorption strongly depend on the accessibility of the surface, in accordance with the flow streamlines. We identify configurations (regions of highest confinement, i.e. contact points between beads) where the adsorption is fully diffusion limited. At early stages of adsorption, these regions can account for up to 10% of the surface of the medium and therefore impact the supposedly known dynamics at global scale.

To go further, we link local observations and global description of the dynamics to discuss the impact of the pore size heterogeneity, at various flow rates (Darcy velocities in the range 0.05 to 9 mm/s). We show the impact of the flow on the heterogeneity of the deposition of the NPs through 1D coverage profiles over time and over the whole sample. Finally, we propose a simple model describing the full beads coverage dynamics over space and time. We can define and decouple a geometric (characteristic deposition length) and a kinetic (characteristic exploration time) components for a complete understanding of the adsorption mechanisms.

References:

1. Lehoux et al. Transport and adsorption of nano-colloids in porous media observed by MRI. Transp Porous Med, 2017
5. Tan KL, Hameed BH. Insight into the adsorption kinetics models for the removal of contaminants from aqueous solutions. Journal of the Taiwan Institute of Chemical Engineers, 2017

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 522

New Capacities for Hydraulic Fracturing Studies: A Full Geomechanical Coupling in a 3D Discrete Fracture Networks

Author(s): Ibtihel Ben Gharbia
Co-author(s): Axelle Baroni; Matthieu Delorme

Corresponding Author(s): ibtihel.ben-gharbia@ifpen.fr

Several unconventional reservoirs have been stimulated using hydraulic fracturing to enhance the production. Further, reservoir simulation technology is facing new challenges in providing key information used for long-term strategic decisions.

To understand and optimize shale reservoirs production, one must capture the role of hydraulically induced fractures, natural fractures and their interaction in the formation. New fractures modify the near field stress inducing the fracture network complexity. Taking into account this changing is essential for improving the well stimulation design (rates, perforations and well locations...) or/and for refracturing operations. Mathematical equations and boundary conditions governing this process and the geomechanical laws are very complex, often requiring significant computational performance. Implementation of such approaches is data intensive and time consuming.

In this work, we focus on the mechanical behavior of fracture networks, to investigate enhancement
new trends in vortex methods for reactive flows

author(s): philippe poncet

co-author(s): laurence hume, jean-mathieu etancelin
This talk will focus on the numerical aspects of reactive flows and pore-scale modeling, and how involving vortex-like methods can substantially improve computational efficiency, that is to say optimize the use of computing resources (computational time and memory storage). After briefly describing the numerical approach, a few numerical simulations of calcite dissolution will be presented.

Vortex Methods are Lagrangian methods -also called particle methods- well fitted to the study of complex transport phenomena[5]. We will first exhibit this feature on bead stacks and their related permeability estimations, and on heterogeneous Xanthan injection in real rock geometries obtained by MicroCT scans[6]. Their hybrid formulation uses high order interpolations between grids and particles, such that adequate numerical schemes are performed either on grids or on particles. The goal is then to compute transport on particles and to use as much as possible fast solvers on grids, in order to minimize the computational time. The penalization method can be included in such schemes[4], making possible to consider arbitrarily shaped body and their dissolution. Consequently, the millimeter scale flow is modeled by the non-linear Stokes-Brinkman equation[3] whose Brinkman term is evolving with a coupling to transport of acid and chemical product.

Concerning reactive flows, three time scales are involved: a hydrodynamic time scale (under the second) in which the flow is able to cross the domain at the pore-scale; a time scale allowing to reach a quasi-stationary reactive state of reaction rate; a dissolution time scale for which the solid body evolves. We will consider the case of a calcite core dissolution at pH=2, in the context of a collaborative study with S. Molins, S. Soulaïne and N. Prasianakis. For this configuration, these three time scales are about 1s, 10s and 1h, respectively.

The numerical method is built specifically with a time-splitting algorithm such that velocity computing and interpolations are performed meaningfully in order to avoid useless computations. In practice we will show that a good strategy is to compute chemistry, diffusion of species and transport on particles, while penalization, velocity computation and viscous diffusion are performed on grids. This strategy decreases the number of interpolations thus improving the computational time. In this spirit, chemistry and hydrodynamics can be considered at different resolutions, and require only a down-scaling of solid concentration. This fits very well to GPU or hybrid CPU-GPU computing, which is currently one of our main developments.

Beyond the multi-scale aspects in time and space, two key points can be mentioned. On the one hand, we will show that time step adaptation can be performed, based on the chemistry evolution (or lack thereof). On the other hand, introducing vorticity unlocks the necessity to make the penalization implicit (usually, explicit penalization has stability issues), which allows the use of fast grid solvers based on Fast Fourier Transforms (FFT), in the spirit of [2]. Finally, several simulations will illustrate how far it is possible to go in terms of resolution and physical time simulated, for Reynolds numbers from 0.24 to 240.

References:


Parallel 5-A / 532

Non-modal growth of perturbations in miscible displacements with non-monotonic viscosity profiles

Tapan Kumar Hota¹ ; Manoranjan Mishra²

¹ Indian Institute of Technology Ropar, India
² Indian Institute of Technology Ropar, Rupnagar, Punjab, India 140 001

Corresponding Author(s): hota.tapan@gmail.com

We study the effect of a non-monotonic viscosity profile on miscible viscous fingering in porous media. This hydrodynamic instability is studied by coupling the continuity and Darcy equations with a convection-diffusion equation for solute concentration that determines the viscosity. A toy viscosity model composed of a sequence of transformation in a sine function is considered. Parametric studies are performed in terms of the end-point viscosity contrast, maximum viscosity, and the corresponding value of the concentration. We employ a non-modal analysis (NMA) based on the singular value decomposition of the propagator matrix approach to perform the stability analysis of the non-autonomous linear system. NMA facilitates to identify the optimal amplification of the perturbations and its spatial structure. We demonstrate that there is a disagreement of previous linear stability analyses and NMA. This disagreement is inherited from the perturbation structure and the parameters involved in defining the non-monotonic viscosity profiles. Our study shows that miscible displacements with non-monotonic viscosity profiles can successfully be analyzed using NMA and paves the way for future work to understand the displacements with a non-monotonic viscosity in miscible reactive flows.

References:
1) Anne De Wit (adewit@ulb.ac.be),
2) Jalel Azaiez (azaiez@ucalgary.ca)
3) Qingwang Yuan (qyuan@ucalgary.ca) Acceptance of Terms and Conditions:

Parallel 4-E / 224

Non-uniform density of gas confined in nanopores.

Author(s): Lucyna Firlej¹

Co-author(s): Bogdan Kuchta ²

¹ University of Montpellier, France
² Madirel, University Aix-Marseille, France

Corresponding Author(s): lucyna.firlej@umontpellier.fr

Unlike macroscopic objects, any system of nanometric size shows characteristics that strongly depend on its size and geometric form. It is the consequence of the fact that the major part of atoms (or molecules) of nano-object is located at its surface, their cohesive energy is smaller than for the atoms in the bulk. Here we show that when a fluid is confined in nano-volume, delimited by non-interacting pore walls, its density is heterogeneous, decreases close to the pore wall, and, on average, is smaller than the density of bulk fluid. The heterogeneity of distribution of fluid density, resulting from the nano-confinement, progressively weakens when the pore size increases, and totally disappears for pores larger than 5 nm. On the other side, in the limit of very small pores, the fluid density approaches
the ideal gas value. This effect should be distinguished from the well known heterogeneity of density of fluids adsorbed in nanopores, driven by the difference between the strength of fluid-fluid and fluid-pore wall interactions, that varies with the distance from the pore wall. The reported observation has non-trivial influence on evaluation of excess/total adsorption in nanopores, as these two quantities are calculated assuming the known – and homogeneous – bulk density of gas in the pore. Additionally, the gas density in the pores depends on the definition of the pore volume which is neither straightforward nor unique. The right estimation of both: pore volume and gas density is essential for quantitative interpretation of experimental adsorption isotherms: evaluation of pore size distribution and of the amount of adsorbed gas. We analyze this problem on an example of five gases: H2, CH4, the two intensively studied energy vectors, and N2, Ar, and Kr, commonly used for characterization of porous structures. For H2, the distributions of densities of gas confined in adsorbing and not adsorbing pores are compared and commented.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 4-F / 709

Nonlinear Safeguarding for Complex Physics; Search-less Line-search

Rami Younis1 ; Giorgiy Lutidze1

1 University of Tulsa

Corresponding Author(s): ryounis@utulsa.edu

This work develops the theoretical basis and practical application of a promising class of safeguarding strategy in the context of the solution of implicit timesteps for multiphase multicomponent flows in general.

While classic globalization methods such as the linesearch for sufficient descent are problem independent, they require numerous computationally costly evaluations of the residual system. Furthermore, they may overly conservative and result in small Newton updates. Developments over the past decade have cemented the efficacy of component-wise relaxation safeguards as an alternative to global search methods, particularly when the relaxation parameter can be deduced from heuristic arguments at constant cost. These methods however are problem specific in the sense that they require prior information about the nonlinearity of the numerical flux over the component space at hand. Recently, the ideas of these component-wise numerical flux analyses were generalized to systems of equations where in essence, a search procedure is used to determine a relaxation length. The result is a return to the need for an expensive search procedure involving numerous residual evaluations. In this work, the criterion for an admissible step along a Newton direction is abstracted; it may be a residual descent criterion, or a local Lipschitz estimate. We apply a discretization error analysis and local functional estimates to then compute the steplength that will satisfy this criterion.

The damping algorithm is based on viewing the Newton iteration as a forward Euler discretization of the Newton flow equations. Three a posteriori local discretization error estimates are derived; the first is an extension of the Poschka method to computably estimate the norm of the derivative of the Newton step with respect to step-length. This relatively costly estimate provides an accurate measure of the departure from the Newton flow path. The second estimate is based on Richardson extrapolation, and the third involves an extended Adams-Bashford method. We propose to control the Newton step length by limiting the estimated local discretization error. The control strategy is conservative far from the solution, and can be shown to result in the standard Newton method otherwise.

Computational results are presented for a series of simulation problems with increasing complexity. First, results for two phase flow simulations demonstrate that the proposed method is competitive with, but not superior to recently proposed trust-region based strategies. For thermal and multicomponent problems the method is compared to classic trust-region and line-search methods. Superior
robustness and computational efficiencies are observed, and the iteration converges for significantly larger time-step sizes.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 212

Nonlinear finite-volume schemes for complex flow processes and challenging grids

Bernd Flemisch$^1$; Rainer Helmig$^1$; Martin Schneider$^1$

$^1$University of Stuttgart

Corresponding Author(s): martin.schneider@iws.uni-stuttgart.de

The numerical simulation of subsurface processes requires efficient and robust methods due to the large scales and the complex geometries involved. To resolve such complex geometries, corner-point grids are the industry standard to spatially discretize geological formations. Such grids include non-planar, non-matching and degenerated faces. The standard scheme used in industrial codes is the cell-centered finite-volume scheme with two-point flux (TPFA) approximation, an efficient scheme that produces unconditionally monotone solutions. However, large errors in face fluxes are introduced on unstructured grids. The authors present a nonlinear finite-volume scheme applicable to corner-point grids, which maintains the monotonicity property, but has superior qualities with respect to face-flux accuracy. The scheme is compared to linear ones for complex flow simulations in realistic geological formations [1,2]. In addition, we present recent developments regarding convergence analysis for a family of nonlinear finite-volume schemes [3].

References:


Click here to agree

Parallel 4-A / 706

Novel bio-organoclay composites designed to seal leaking wellbores

Andres Clarens$^1$; Fangwei Cheng$^1$; Lisa Colosi$^1$

$^1$University of Virginia

Corresponding Author(s): andres@virginia.edu
Emissions of methane and other hydrocarbons from old or abandoned oil and gas wells are a growing environmental and public safety risk. There is growing interest in identifying materials that are inexpensive and can be easily pumped into the wellbore from above in order to create a permanent seal for leaking hydrocarbons. Here we developed a novel bio-clay composite (BCC) material with the capability of swelling in the presence of methane. Conventional bentonite clays swell significantly in water, which would limit the ability of these materials to penetrate deep into the wellbore. In contrast, modified organoclay materials swell poorly in the presence of light chain hydrocarbons like methane. BCCs leverage the growth of microbial organisms such as methanotrophs that metabolize the methane and produce biomass. The growth of these microorganism will result in the accumulation of biomass, which in turn will induce the swelling of the BCCs.

In this talk we will report on experimental results carried out over the past year to characterize this approach. The novel BCCs were synthesized by reacting sodium bentonite clay with amino acids using ion exchange process. Conventional organoclay materials are typically made using quaternary ammonium compounds and other surfactants but these tend to have biocidal properties. The result of this synthesis was a hydrophobic organoclay that was biocompatible. To evaluate the performance of these BCCs we used E. coli as a model microbial organism. Inhibition tests of E. coli growth by amino acids were conducted wherein cells were exposed to different concentrations of amino acids and a positive control, and the bacterial growth was recorded by measuring their optical density. The results of inhibition tests showed that amino acid-based BCCs have insignificant impacts on the growth of E coli. We also conducted swelling tests and hydraulic conductivity tests to understand how biogenic solution will impact the swell index and permeability of BCCs. BCCs were characterized using small angle X-ray scattering (SAXS) to identify the d-spacing of the samples before and after being mixed with biogenic solution. The results demonstrated that the introduction of biomass creates higher swelling index and dramatically reduced hydraulic conductivity for BCCs.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-G / 741

Novel finite-volume methods for anisotropic linear elasticity and poromechanics problems with full tensors

Kirill Terekhov¹ ; Nicola Castelletto² ; Hamdi Tchelepi²

¹ INM RAS
² Stanford University

Corresponding Author(s): tchelepi@stanford.edu

We propose a novel finite volume method for anisotropic linear elasticity problem. The derivation of the flux approximation method for elasticity problem closely follows our previous work on the nonlinear finite volume methods for diffusion equation featuring positivity and discrete maximum principles. It is based on the extensions of the harmonic point idea of [2] from the scalar to vector equations. We further extend the idea to coupled anisotropic flow and mechanics, featuring full tensors for permeability, Biot coefficient and stiffness tensor. Both methods handle star-shaped polyhedral grids, admit the construction of nonlinear finite volume methods and yield several new research directions.


References:
Poster 3 / 559

Nuclear Magnetic Resonance Relaxation and Diffusion Measurements to Monitor Phase Changes in Hydrates

Author(s): Linn W. Thrané
Co-author(s): Joseph D. Seymour, Sarah L. Codd

1 Mechanical and Industrial Engineering, Montana State University
2 Chemical and Biological Engineering, Montana State University
3 Mechanical and Industrial Engineering

Corresponding Author(s): linn.thran@montana.edu

State of the art multi-dimensional nuclear magnetic resonance (NMR) relaxometry and diffusometry techniques along with magnetic resonance imaging (MRI) are applied to explore and characterize phase change in complex systems. High-field NMR techniques are highly sensitive to the thermodynamic phase of the system as well as restrictions on molecular motion. High resolution imaging along with T1-T2 relaxation correlation experiments and pulsed gradient spin echo (PGSE) NMR methods are demonstrated to characterize hydrate formation. The NMR techniques are applied to monitor the hydrate formation process in a model water-cyclopentane system at various sub-cooling temperatures. Using T1-T2 correlation NMR, the transition from mobile to restricted dynamics is observed simultaneously for both water and cyclopentane throughout the formation process by examining the magnetization decay as a function of T1 at multiple T2 times. Spectrally resolved diffusion measurements allow monitoring of the hydrate formation process by measurement of the area under the liquid water peak as it disappears due to solidification of the water in the hydrate. Also, restriction in diffusive motion due to boundaries between solid-liquid or immiscible liquid-liquid phases provides a means to characterize structure by the size of particles or pore spaces. Magnetic resonance imaging (MRI) data monitors total hydrate formation rate based on cyclopentane saturation and temperature, as well as the spatial heterogeneity within the system. The combination of these MR techniques allows for exploration of the complex molecular dynamics involved in hydrate formation processes.

References:

Acceptance of Terms and Conditions: Click here to agree

Parallel 10-B / 528

Numerical Model of a thermochemical heat storage reactor

Author(s): Gabriele Seitz
Co-author(s): Holger Class, Rainer Helmig

1 University of Stuttgart

Corresponding Author(s): gabriele.seitz@iws.uni-stuttgart.de

Thermochemical heat storage has a large potential due to its high storage density. In the range of high to medium temperature heat storage the system Calciumoxide – Calciumhydroxide is of
special interest, as it reacts at handable temperatures (300-500 °C), is environmentally friendly and financially attractive.

The following chemical reaction is considered:

\[ \text{CaO}_s + \text{H}_2\text{O}_g \rightarrow \text{Ca(OH)}_{2,s} + \Delta H_R \]

In order to develop a technical application, the processes of the chemical reaction have to be investigated: The granular material (\(\text{Ca(OH)}_2 / \text{CaO}\)) undergoes a volume change so that its porosity and permeability and thus the flow processes of the water vapor are changed. Furthermore, the reaction kinetics and the cycling stability have to be examined.

To understand the processes and estimate their relevance on the different scales, a numerical model is built in the open-source simulator DuMuX. The constitutive relations of the complex system are depicted in a multiphase system. Changes in the structural properties such as porosity and permeability are considered. Emphasis is further put on the formulation of the energy balance.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-E / 156

Numerical Modelling of Reactive Flow and Wormhole Formation in Carbonate Rocks

Jun Yao\(^1\)

\(^1\) China University of Petroleum, Qingdao

Corresponding Author(s): yaojunhp@126.com

Many subsurface operations – such as drilling, cementing, well completion, and production – can result in damage to the rock formation near the wellbore, decreasing the permeability and resulting in a reduction in oil or gas production. Acidizing is one type of treatment that is employed to increase the permeability around the wellbore. In carbonate rocks, acidizing can not only reduce the damage, but it also can create conductive channels that extend some distance into the rock mass, known as wormholes, whose hydraulic conductivity is several orders of magnitude larger than that of the porous medium. Moreover, the experimental observation has shown that the amount of acid required to breakthrough is minimum when wormhole dissolution is formed. Therefore, simulating the reactive flow in carbonate medium and finding the optimum injection rate are of fundamental importance to reduce the acidization cost. In this work, a two-scale continuum model is improved and extend to the 3-D radial flow condition, and used to simulate reactive flow and wormhole formation in carbonate rocks. Then, combining the two-scale continuum model and the discrete fracture network model, a continuum model is developed that is used to examine wormhole formation in cases with single and multiple fractures, including characteristics such as fracture orientation, pattern and aperture. Because of the positive feedback associated with fractures, the simulation results indicate that the flow-dissolution process typically uses only some of the available fracture pathways.

References:

Numerical Simulation Study on Pore Scale Seepage of Porous Media Based on Finite Volume Method

Shuo Wen¹ ; Dongxu Han² ; Yajun Deng³ ; Bo Yu² ; Dongliang Sun²

¹ Beijing Institute of Petrochemical Engineering
² School of Mechanical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, China
³ China University of Petroleum,Beijing

Corresponding Author(s): 18800104597@163.com

Abstract: The numerical simulation of pore scale seepage in porous media is of great significance for the development of new energy sources, such as shale gas and geothermal energy. In the past few years, many scholars have developed the numerical method including finite volume method (FVM), Lattice Boltzmann Method (LBM) and molecular dynamics to achieve this simulation in different levels. It is easy for us to understand the basic idea of FVM, and then we can give a direct physical explanation for the above phenomena. FVM has stronger advantages in CFD (computational fluid dynamics) since the conservation law is meet in the whole computational domain. Based on the FVM, a large number of models on multi-phase flow and non-Newtonian fluid have been developed and it has showed more advantages in the aspect of solving complex pore flow problems. However, there are two shortcomings in the process of using FVM: (1) Due to the complexity of the pore geometry in the porous media and irregularly curved pore walls, the quality of the generated grid is not high; (2) It is relatively difficult to deal with a large number of pore boundaries in the porous media. To cure the above problems, a simple processing method is proposed as follows in this paper: On the one hand, in porous medium, both the penetrating space and solid frame are regarded as the fluid region, while, to describe solid boundary approximately, the viscosity of the solid skeleton structure is set to infinite. On the other hand, the whole region is discretized through the Cartesian orthogonal grid and the Immersed Boundary Method(IBM) is adopted to describe the smooth and complexed boundaries between the penetrating space and solid frame. In this paper, the proposed method stated above is conducted on OpenFOAM by the finite volume method in which the convection term is discreted in the QUICK scheme. After that, the corresponding systematic evaluations of the proposed method are performed and results illustrate that the method is of great accuracy and robustness. It can be used to study the flow in complex porous media.

References:

Parallel 10-H / 707
Numerical Simulation of Carbonate Matrix Acidizing Using Adaptive Enriched Galerkin Method

Author(s): Rencheng Dong

Co-author(s): Sanghyun Lee ; Gergina Pencheva ; Mary Wheeler

1 The University of Texas at Austin
2 Florida State University

Corresponding Author(s): rencheng_dong@utexas.edu

Matrix acidizing is a stimulation technique that is extensively being employed by petroleum industry in carbonate reservoirs to improve permeability and enhance production [3]. The acidizing technique involves injecting acid to dissolve minerals in order to create long highly conductive channels known as wormholes. The wormhole formation is the optimal scenario in carbonate matrix acidizing. Intensive chemical reactions and pore structure changes mainly occur near the acid front. Predicting these wormholes and the performance of carbonate acidizing is challenging due to the multi-scale heterogeneous properties of carbonate reservoirs and complicated rock-acid chemical reactions.

One of the classical methods employed in the acid transport is the first-order finite volume method on static mesh. However, the numerical solution exhibits diffusive acid fronts and the method requires very fine mesh to resolve wormholes. Here we employ a two-scale continuum model proposed in [3] for the matrix acidizing problem. To simulate wormholes more accurately and efficiently, we develop a new numerical simulator for acidizing using an adaptive enriched Galerkin finite element method (EG) [4,1,2]. The EG is formulated by enriching the conforming continuous Galerkin finite element spaces with piecewise constant functions. EG is a high-order method with less numerical dispersion and grid orientation effects than standard finite difference or finite volume methods.

The flow and transport equations are solved sequentially using EG. Entropy viscosity stabilization method [2] is used to prevent any non-physical acid concentration. Entropy residual is used as a posteriori error indicator to dynamically refine the mesh near the moving wormhole interface. Entropy residual stabilization is a very efficient technique to avoid spurious oscillations of the high-order EG method and capture sharp acid fronts for the reactive transport problem.

Several numerical examples are presented, which reproduce different dissolution patterns observed in previous laboratory experiments under different acid injection rates. One of the main advantages of the proposed adaptive EG method is that it reduces the number of degrees of freedom in the non-computationally-intensive areas, hence reduces the simulation runtime, while still capturing the wormhole formation.

References:

Click here to agree
Parallel 3-F / 636

Numerical Simulation of Nanoparticle effects on Multi-phase System Dynamics

Author(s): Rasoul Arabjamaloei

Co-author(s): Milana Trifkovic ; Steven Bryant

1 Assistant Professor
2 Professor

Corresponding Author(s): steven.bryant@ucalgary.ca

Solid nanoparticles (NPs) have shown promise to play a major role in novel enhanced oil recovery methods by altering reservoir wettability, reducing interfacial tension and increasing mobility ratio. Solid nanoparticles could be implemented as emulsion stabilizing agents in combination with surfactants and polymers. Stabilized emulsions are a desired state in enhanced oil recovery. In this study, the contribution of NPs in hydrodynamics of multi-phase systems including their effect on interfacial tension and mobility ratio was studied. The free energy Lattice Boltzmann Method was used to solve the Cahn-Hilliard convection-diffusion and the Navier-Stokes equations in a two-dimensional Cartesian domain. The NPs were added to the system as point particles with zero volume. A potential function was assumed to represent the chemical potential alteration of the multi-phase system due to the presence of NPs. Attractive and repulsive interaction of the NPs was entered into the model by Morse potential function. The results of spinodal decomposition showed that different types of emulsions (oil in water, water in oil, water in water) could form at the presence of particles with different wettabilities. The effect of the presence of NPs in a capillary tube on contact angle was studied and it was observed that low concentration of NPs does not significantly affect the contact angle. The process of suspended droplets getting coated by neutral-wet NPs was simulated and it was observed that attractive interaction of NPs would result in multiple layers of coating. The Collision and coalescence of two droplets at the presence of different type of NPs was simulated and it was observed that neutral-wet NPs dominate the collision hydrodynamics at high NPs concentrations. It was also observed that the nanoparticles with repulsive forces would stabilize emulsions at lower concentrations comparing to nanoparticles with attractive forces. This work showed that the free energy Lattice Boltzmann method combined with NPs assumed as points is an effective tool to model and simulate the hydrodynamics of multi-phase systems in micro and nano scales. The computation cost of the simulation was also discussed in details.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-H / 455

Numerical Study on the Influence of Natural Fracture Size on Heat Transfer Process in Hot Dry Rock

Kangxin Zhang ; Dongxu Han ; Bo Yu ; Dongliang Sun ; Jingfa Li

1 China University of Petroleum, Beijing
2 School of Mechanical Engineering, Beijing Institute of Petrochemical Technology, Beijing 102617, China
3 Department of Petroleum Storage and Transportation Engineering Beijing Institute of Petrochemical Engineering

Corresponding Author(s): cupzkx@foxmail.com

Geothermal is a kind of unconventional energy with abundant reserves. It owns the advantages of low carbon emissions, climate-free, widely distributed, and enormous mining potential. At present, the research on the development of hot dry rock (HDR) are mainly studied from the perspective of
the macroscopic scale. However, due to the existence of natural fractures of different scales in real rocks, these studies find it is a great challenge to obtain the seepage and heat transfer laws of the heat transfer medium in the fracture. For this reason, the rock porosity porous media model with different porosities is constructed by QSGS method in this paper, and the numerical simulation is carried out with the Lattice Boltzmann Method. To verify whether the construction method of porous media has effect on the calculation results, several porous media structures method are adopted for comparison. According to the mesoscopic simulation results, the seepage heat transfer laws of three kinds of fractures with different sizes are found to be quite different. For further study the influence of seepage flow with different fracture sizes on the heat transfer process, the porous media model is divided into three categories according to the natural fracture size. After the three kinds of fractures are blocked respectively, the Lattice Boltzmann Method is implemented and the results are compared and analyzed. The results illustrate that the heat transfer of micro fracture can be represented by the correction coefficient, this correction method can ignore the complex seepage characteristics of micro channel and reduce the calculation burden. The method presented in this paper is of great importance to the simulation of the hot dry rock development with large computational area.

References:
Click here to agree

Poster 1 / 745

Numerical analysis of viscous oil recovery using micromodel experiments on thermal solvent-based displacement

Author(s): Marelys Mujica

Co-author(s): Igor Bondino ; Igor Bogdanov

1 CHLOE, University of Pau
2 Total
3 laboratoire CHLOE, Université de Pau

Corresponding Author(s): marelys.mujica@univ-pau.fr

Hot solvent injection is an in-situ technology which uses heated solvent for efficient and sustainable viscous oil (VO) recovery (cf. 93 kg per barrel less GHG emission than SAGD technology). The process reduces the oil viscosity via mass and heat transfer so that the combined effect of heating and solvent dilution yields a better result than in steam (SAGD) or cold solvent injection (VAPEX) cases.

In this case, the injection of the solvent in gaseous state reduces the amount of solvent required per unit volume of produced oil, and takes advantage of higher rate of solvent diffusion. The solvent will not remain in gaseous state but will condense downstream and release a latent heat making easier its mixing with the VO in-place due to the local temperature increase. Recently the hot solvent injection technology (known also under the name NSolv) had its first successful pilot project designed to recover bitumen from oil sands.

Physically speaking the VO displacement in the solvent-based process is a complex combination of dynamic energy and mass transport and phase transformation phenomena. The rapidly emerging experimental technique of fluid dynamical measurements and observations on micromodels (MM) is proved to be a powerful mean providing quantitative information on multiphysical processes in porous media.
The numerical simulation of solvent injection for VO displacement in a MM setup has demonstrated its feasibility and usefulness both for model design and experimental results analysis. This includes first a pore-scale imaged-based study of micromodel transport properties. Then the Darcy-scale model has been developed and applied for dynamic displacement study. It has been shown that although being not capable to reproduce in detail the fluid- and thermodynamic diversity of the displacement (especially at pore scale), the developed numerical model has indicated the process key parameters and offered the framework for their quantitative determination.

Finally the dedicated study of process dynamics and corresponding adaptation of the numerical model parameters has been presented and discussed.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 975

Numerical investigation of adsorption and slippage effects on unconventional gas transport in shale reservoirs using molecular dynamics and reservoir simulations

D.-J. Youn; Yiteng Li; Shuyu Sun

1 King Abdullah University of Science and Technology

Corresponding Author(s): dongjoon.youn@kaust.edu.sa

Gas transport in an unconventional reservoir is a complicated process that is highly subject to non-linear multi-physics phenomena, such as gas molecule’s sorption and slippage effects especially in tiny pores. The quantity of the adsorbed gas release and gas permeability changes due to the complex gas transport phenomena can significantly affect the entire production in unconventional reservoirs. In this research, we analyze these two gas transport mechanisms in shale matrix with different reservoir conditions by molecular dynamics (MD) simulation. A dual control volume grand canonical MD is applied to estimate methane molecular adsorption/desorption and slippage effects in nanometer-scale pores in terms of Langmuir isotherm (pressure and temperature) and Klinkenberg b-factor with different pore sizes and reservoir conditions. Furthermore, these parameters are implemented into a double porosity (DP) reservoir model to determine their effects on the overall gas transport behavior and production efficiency in reservoir-scale. In this paper, we describe the details of the computational models, MD and DP, and example studies to show the applicability and capability of our models to analyze the various fluid transport mechanisms in both pore- and reservoir-scale simulations.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 338

Numerical methods for non-equilibrium porous media flow models

Iuliu Sorin Pop; Stefan Karpinski; Xiulei Cao; Florin Radu; Hans van Duijn; Koondanibha Mitra

1 Hasselt University
Standard models for flows in porous media assume that quantities like saturation, phase pressure differences, or relative permeability are related by monotone, algebraic relationships. These relationships are determined experimentally, assuming that the involved quantities have reached a local equilibrium. Under such assumptions, the solutions of the resulting mathematical models have properties like stability in various norms, and satisfy the maximum principle. In particular, standard models rule out effects like saturation overshoot or the formation of finger profiles, which have been evidenced experimentally. This contradiction is the main motivation when considering non-equilibrium models, where dynamic effects are included in the above mentioned relationships. The resulting models are nonlinear evolution systems of (pseudo-)parabolic and possibly degenerate equations, and may involve differential inclusions. In this contribution we discuss different numerical schemes (multipoint flux approximation, discontinuous Galerkin) for approximating the solution of non-equilibrium models. In particular, we present the rigorous convergence analysis of the numerical solution to the weak solution of the model. Also, we analyze different linear iterative methods for approximating the numerical solution to the nonlinear, fully discrete problems encountered at each time step.

References:

Click here to agree

Parallel 8-H / 264

Numerical modeling and simulation of two-phase flow problems in heterogeneous porous media with gravity and dynamic capillary pressure

Paola Ferraz¹ ; Jardel Vieira² ; Eduardo Abreu³

¹ University of Campinas - Sao Paulo - Brazil
² University of Campinas - Sao Paulo - Brazil
³ University of Campinas, Sao Paulo, Brazil

Corresponding Author(s): eabreu@ime.unicamp.br

Numerical simulations of immiscible two-phase flow in porous media with dynamic capillary pressure and gravity interactions in heterogeneous porous media are presented with a novel computational method based on ideas introduced in [1]. We formulate and test numerically a new two-dimensional fully coupled and implicit procedure
for numerically solving two-phase transport problems of pseudo-parabolic nature, see [1,2,3]. For the parameter range considered, immiscible viscous fingers are found to undergo interaction with dynamic capillary pressure and gravity effects for typical flow path situations in porous media transport problems. The dominant feature for these flows is the saturation overshoot under non-equilibrium effects in the capillarity pressure [2,3]. Our numerical experiments demonstrate the viability of the proposed procedure for multiscale problems in heterogeneous high contrast media.


References:


Click here to agree

Parallel 4-F / 449

Numerical recipes for problems involving highly contrasted capillary pressures

Joubrine Aghili¹ ; Konstantin Brenner² ; Julian Hennicker³ ; Roland Masson⁴

¹ University Côte d’Azur, LJAD-Inria-CNRS
² LJAD, Université de Nice Sophia Antipolis
³ University of Geneva
⁴ LJAD

Corresponding Author(s): konstantin.brenner@unice.fr

This contribution deals with numerical simulations of immiscible two-phase flow in heterogeneous porous media. The hydrodynamic properties of the geological porous media are naturally discontinuous at the Darcy scale, which has to be accounted for by discretization methods. In this talk we focus on handling extreme heterogeneities in the capillary pressure/saturation relation arising, in particular, in the context of flow in fractured media. In order to properly account for saturation jumps at the rocktype interfaces the supplementary unknowns are introduced at such interfaces. We investigate and compare two strategies for solving the discretized two-phase flow equations. The first approach, suitable for cell-based finite volume methods, relies on the nonlinear elimination of the interface dofs, which will lead us to prove existence and uniqueness (in a certain sense) of solution to the local interface problem. The second approach is based on a judicious choice of primary unknowns at the interface. It does not requires the elimination of the interface dofs, and thus can be extended to vertex-based methods.
Numerical simulation of proppants transport and placement in fracture

Hai Sun¹; xiaoyu Wang¹; Yao Jun¹; Yongfei Yang²

¹ China University of Petroleum (East China)

Corresponding Author(s): sun_hai123@sina.com

The two-phase flow study is meaningful for mass transfer in various industrial processes, for example the prediction of proppant distribution is of significance due to the fact that proppant placement contributes to the enhanced production of fluids by affecting the conductivity of the fractured reservoir. Since it is difficult and expensive for experiments to consider various conditions and detect the movement of every particle, numerical simulation methods are often applied. For more precise simulations, the simplified fracture geometry and soft sphere particle model is used. The coupled CFD-DEM (Computational Fluid Dynamics-Discrete Element Method) approach is implemented in this work to compute proppant transport and settlement in a specific configuration. The DEM is employed to assess particle-particle and particle-geometry interactions, while the CFD is used to describe the flow field. The comparison of simulation results shows that the profile of the particle bed produced by the CFD-DEM is consistent with those derived from experiments. The proppant motion is captured in detail during transport to interpret the transport mechanism at the particulate scale. Once separated from the suspending layer, particles first accelerate, then decelerate, with dramatic rolling; meanwhile, both velocity and angular velocity slow down and finally stop. The asymmetry of fractures in the vertical direction is common due to lithologic heterogeneity. The effect of the injection position cannot be neglected. Thus, cases where particles of different densities are injected at three different injection heights are simulated. It is shown that the separation of particles is conditional and the difference in density is not the dominant factor. This separation is the most obvious, and the area covered is maximized, when low-density particles are injected from a higher inlet.

References:
Acceptance of Terms and Conditions:
Click here to agree

Numerical simulation of two-phase flow properties in rough fractures considering the normal deformation

Dongying Wang¹; Jun Yao¹; Hai Sun¹; Yongfei Yang¹; Wenhui Song¹

¹ Research Centre of Multiphase Flow in Porous Media, China University of Petroleum (East China), Qingdao, China

Corresponding Author(s): wdy_upc@126.com

Stress-dependent permeability and capillary force play important roles in determination of flow characteristics in fractures. Traditional empirical equations for relative permeability cannot accurately reflect transport behavior in rough fractures in consideration of normal deformation. In this paper, a systematic approach has been proposed to determine flow properties, such as relative permeability, capillary force, and the relationship between normal stress and flow properties in rough fractures.
based on the percolation theory. The rough fracture was described as a two-dimensional model, characterized by aperture as a function of position in the fracture plane. On the basis of Gaussian aperture distributions and cubic law in local parallel plate model, capillary force and relative permeability versus wetting phase saturation for both wetting and non-wetting phase were predicted in closed form, and the influence of normal deformation on fluid transport was investigated by decreasing the mean value of Gaussian aperture distributions. Numerical simulation results imply that the two-phase flow properties including the relationships between relative permeability, capillary force and wetting phase saturation depend sensitively on the normal deformation and spatial aperture distributions. Furthermore, a series of experiments data were applied to validate our numerical simulation results.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-F / 579

Numerical simulation of wicking in porous media

Dawid Zimnik1; Michael Dreyer2

Corresponding Author(s): dawid.zimnik@zarm.uni-bremen.de

Phase separation and the vapor free delivery of liquids is a challenge in a compensated gravity environment. Porous materials are used for liquid and vapor phase separation. They enable the transport (wicking) of liquid and provide a barrier against penetrating gas (bubble point). The wicking process is the imbibition of liquid into porous structures due to capillary forces. To predict the liquid behavior inside porous materials, numerical simulations on the macroscopic level can be performed. The macroscopic parameters – porosity, pore radius and permeability – have to be known to perform macroscopic simulations. For this purpose, a real sample was scanned using X-ray tomography and a 3D model was reconstructed from it. CFD simulations were performed on the pore level using a 3D model and an appropriate representative volume element (REV) to determine the macroscopic parameters.

References:
Click here to agree

Poster 1 / 951

Numerical study of effective thermal properties of granular porous medium using Lattice Boltzmann methods

Muhammad Fowaz Ilkma1; Roohollah Askari2; S. Hossein Hejazi3; Yongfei Yang4; Jun Yao5

1 Subsurface Fluidics and Porous Media Laboratory, Department of Chemical and Petroleum Engineering, University of Calgary, Calgary, Alberta, T2N 1N4
2 Department of Geological and Mining Engineering and Sciences, Michigan Technological University, Houghton, Michigan, 49931-1295
3 Center of Multiphase Flow in Porous Media, School of Petroleum Engineering, China University of Petroleum Engineering (Huadong)

Corresponding Author(s): mfikram@ucalgary.ca
Heat conduction in granular porous media is a phenomenon that is relevant to a broad spectrum of problems in science and engineering disciplines including physical, earth, and biological sciences, to name a few. Effective thermal conductivity in granular porous media is a function of morphological features of the medium such as grain shape, grain size, and geometrical structure. Thermal contact resistance can also affect heat conduction due to topological features such as the surface profile of the grain. Furthermore, the compressive pressure and presence of different fluids in the pore space along with partial saturation can also dictate the nature of the effective thermal properties.

To study the effect of all these factors on the effective thermal conductivity of granular porous medium, we simulate heat conduction by developing a two-dimensional, parallel and thermal Lattice Boltzmann Method (T-LBM) simulator using existing open-source libraries. We use this simulator on a digitally reconstructed, two-dimensional granular porous medium that is generated with an existing packing algorithm. We then conduct a progressive investigation by first, introducing thermal contrast resistance as surface roughness on the grains and study its effect on thermal conductivity. Second, we introduce thermal anisotropy in the system by inclusion of elliptical grain packing in the medium. Third, we investigate the effect of partial saturation of water and air in pore space. We use an LBM single component multiphase model to simulate phase segregation in the pore space. We also incorporate elastic deformation of grains based on an existing model, which depicts the surface topology of grains as a self-affine fractal function. This elastic deformation is a function of Young’s modulus of the grains and the external compressing pressure.

Based on our investigation, we observe that thermal contact resistance due to the surface roughness of grains reduces effective thermal conductivity. Elliptical packing of grains, manifest thermal anisotropy in the system and causes local heat flux deviations especially when the grain orientation angle changes. External compressive pressures cause elastic deformation of the grain surface and enhance the thermal conductivity of grains with lower Young’s modulus. Introducing partial saturations of water and air in the pore space offsets the effective contribution in heat conduction from the grains as well as the effect of compressing pressure. All of these observations are further accentuated if the thermal contrast ratio of the granular porous medium is changed. We also compare results for selected observations for consistency. A qualitative agreement is obtained with the existing experimental data.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 742

Oil/water two-phase slip flow in a random pore network of shale

Ronghao Cui¹ ; Qihong Feng¹ ; Sen Wang¹ ; Wei Zhang¹

¹ China University of Petroleum (East China)

Corresponding Author(s): ronghaocui1993@163.com

In contrast to the conventional reservoirs, shale reservoirs embody micro-pores developed from inorganic minerals and nano-pores developed from organic matters, which can both exert an important influence on two-phase flow properties. Through a bimodal pore-size distribution (PSD) in whole shale system verified by nitrogen absorption tests may be assumed as the Gaussian mixtures, the random pore-network model for shale is developed with a classification algorithm that decouples the different distributions of inorganic pores and organic pores. Corresponding throats can be generated and distinguished appropriately.

As for shale system, traditional Hagen-Poiseuille flow equation may not be applicable on account of the slip effect in nanopores and pore geometry in the whole system. Here, computational fluid dynamic (CFD) method is utilized to modify bulk/corner phase flow equations in various geometric pores (circular, square, equilateral triangle) for two-phase slip flow. Developing new flow equations, we can estimate the flow characteristics such as capillary pressure and relative permeability relationships in a shale network through the quasi-static simulation technique. Our study confirms the slip effect would significantly affect oil/water two-phase flow in shale. And then, we employ this multiscale network model to further study the influence of shale pore structure on oil/water two-phase flow properties.
Through coupling the multiscale pore-network model and oil/water two-phase slip flow for shale reservoirs, we believe this work can furnish a great importance to the further research associated with flow mechanism in shale.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-C / 281

On Determining the Onset of Asphalt Precipitation using Electrical Conductivity Measurements

Muhammad Sahimi

1 University of Southern California

Corresponding Author(s): msahimi33@gmail.com

An important and largely unsolved problem is accurate prediction of the onset of precipitation of heavy organic compounds, such as asphalts, on the surface of the pores of a porous medium, such as oil reservoir. It was suggested some time ago that an effective method of identifying the onset may be through measuring the electrical conductivity of the solution that contains the heavy organic compounds. We test this hypothesis by carrying out computer simulation studies of asphalt flocculation and precipitation processes, utilizing two models of asphalt formation that have been suggested in the past, namely, those that are based on diffusion-limited and reaction-limited aggregation processes. The simulations model the evolution of the asphalt aggregates as the precipitation agent is added to the solution, and computes the electrical conductivity of the solution as a function of time and the concentration of the asphalt aggregates.

The results indicate that, regardless of the aggregation model, under certain conditions the points at which the aggregates begin flocculating and precipitating induce discernable changes in the conductivity of the solution at particular points. The same changes are detectable in the number of the asphalt aggregates in the solution. However, the changes happen only if the concentration of the asphalt in the solution is relatively high. Otherwise, the electrical conductivity of the asphalt-containing solution exhibits no special feature and, therefore, its measurement is not an accurate method for identifying the onset of asphalt precipitation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-A / 932

On an evolving non-isothermal reactive upscaled model in a porous medium

Kundan Kumar1; Carina Brinddal2

1 University of Bergen
2 Hasselt University

Corresponding Author(s): kundan.kumar@uib.no

For a non-isothermal reactive flow process, effective properties such as permeability and heat conductivity change as the underlying pore structure evolves. We investigate changes of the effective
properties for a two-dimensional periodic porous medium as the grain geometry changes. We consider specific grain shapes and study the evolution by solving the cell problems numerically for an upscaled model derived in Bringedal et al.[2]. In particular, we focus on the limit behavior near clogging. The effective heat conductivities are compared to common porosity-weighted volume averaging approximations. The resulting macro-scale equations are tested on a case where the geochemical reactions cause pore clogging and a corresponding change in the flow and transport behavior at Darcy scale. As pores clog the flow paths shift away, while heat conduction increases in regions with lower porosity.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-B / 860

On modeling partially-saturated flow of a liquid in multilayered thin swelling porous media

Ahmed Kafel\textsuperscript{No}\textsuperscript{r}, Krishna Pillai\textsuperscript{1}

\textsuperscript{1} University of Wisconsin Milwaukee

Corresponding Author(s): kafel@vt.edu

Understanding fluid flow and deformation processes in thin swelling porous media is critical for developing superior consumer absorbent hygiene products such as wipes, paper towels, feminine pads and diapers [1-4]. Fluid-flow models have proven very valuable for the development of these products and have led to the development of fundamental understandings in transport mechanisms, numerical simulation tools, computation infrastructure and lab methods for both characterizing absorbent materials as well as validation of flow and deformation models. In this study we developed a quasi -2D averaged macroscopic mass balance model, based on the volume averaging approach [5-17], for modeling partially-saturated flow of a liquid in multilayered thin, absorbing swelling porous media. In order to describe the absorbency process in [18], fast and accurate simulations with this model are carried out to predict the time and spatial behavior of variables such as piezometric head, saturation, porosity, and layer thickness, and to understand the flow and storage of a liquid in conjunction with the layer deformation. This model enormously improved the computational speeds, allowing to develop a fast and reasonably accurate simulation of the unsaturated flow at lower cost. The numerical results of the simulations predicted well the flow fields of both liquid and solid phases and were in good agreement with the experimental and previous numerical results.

References:


18. Feldkamp, J.R., A mathematical description of liquid flow through partially saturated deformable porous media. report 2.02(TL No 7439.).

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Poster 4 / 878**

**On sugar alcohol based heat storage materials: A nanoscale study and beyond**

David Smulders¹; Camilo Rindt²; Silvia Neda³; Bobby Zhang³

¹ Eindhoven University

**Corresponding Author(s):** d.m.j.smeulders@tue.nl

Batteries and pumped hydropower plants store solar energy in the form of chemical and mechanical energy. Another attractive option is storing energy in the form of heat. Probably the best-know example are the so-called heat pads that are used in outdoor activities. We investigate how to use sugar alcohols as heat batteries. Sugar alcohols are an abundant product of the food industry and they come in many different types. Xylitol for example, is often used in chewing gum. The heat is stored when the sugar alcohol melts and released again upon crystallization. This crystallization
can be at much lower temperatures than the melting which is called undercooling. Undercooling thus allows to store energy without the need for insulation. However, the heat conduction in sugar alcohols is low, limiting the heat power. Also, the crystallization behavior is unpredictable which complicates the storage system design.

Using a nanoscale modeling method, the sugar alcohols are studied in full atomic detail. From the movement of atoms, many material properties are derived that were so far unknown. By adding small amounts of carbon nanostructures to the sugar alcohols, the thermal conductivity of the carbon-sugar alcohol composite was hugely increased. The research also identified two distinct nanoscale heat transfer algorithms, one of which proved to be applicable to the composite material. We also developed a novel method to calculate the solid-liquid interfacial free energy, a key parameter that controls the nucleation and crystallization processes.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 195

On the Examination of the Darcy Permeability of Soft Fibrous Porous Media; New Correlations.

Zenghao Zhu¹ ; Qiuyun Wang¹ ; Qianhong Wu¹

¹ Villanova University

Corresponding Author(s): qianhong.wu@villanova.edu

In this presentation, we report a novel experimental approach to investigate the compression-dependent Darcy permeability of soft porous media. Especially, we are proposing new correlations that describe the change of the permeability of random fibrous porous media as a function of its compression. A special device was developed that consisted of a rectangular flow channel with adjustable gap thickness ranging from 3 mm to 20 mm. Air was forced through the thin gap filled with testing fibrous materials. By measuring the flow rate and the pressure gradient, we have successfully obtained the Darcy permeability of different fibrous porous materials at different compression ratios. Theoretical or semi-empirical models have been compared with the experimental results, indicating various degrees of disagreement. The new correlations were then proposed which fit with experimental data very well. The study presented herein provides a useful approach to evaluate the change of the permeability of fibrous porous media as a function of its compression. It will be valuable for examining fluid flow in fibrous porous media where the permeability is difficult to be measured directly. This kind of porous media widely exists in biological systems.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-B / 432

On the Pressure Generation anRelaxation in a Porous Media under a Spherical Loading Surface

Qianhong Wu¹ ; Qiuyun Wang¹ ; Rungun Nathan² ; Zenghao Zhu¹

¹ Villanova University

² Penn State Berks
Corresponding Author(s): rungumnathan@yahoo.com

The phenomenon of pressure generation and relaxation inside a porous media is widely observed in biological systems. For example, the pressurization inside the cartilage plays the key in the load bearing and lubrication of the knee joints. In this paper, we report a biomimetic study to examine the transient pressure distribution inside a soft porous layer when a spherical loaded surface suddenly impacts on it. A novel experimental setup was developed that includes a fully instrumented spherical piston with supporting structures, and a soft fibrous porous layer underneath. The materials were precisely characterized on their porosities, pore sizes, fiber stiffnesses and permeability. Extensive experimental studies were performed with different porous materials, different loadings and different sized loading surfaces. The pore pressure generation and the motion of the loading surface were recorded by pressure transducers and laser displacement sensors, respectively. A novel theoretical model was developed to characterize the process of the pore pressure generation and relaxation underneath the loading surface and inside the undeformed surrounding materials. Excellent agreement was observed between the experimental results and the theoretical predictions. It clearly demonstrated that the hydrodynamic similarity between porous media on different scales are governed by the Brinkman parameter, \( \alpha = h/K_p^{0.5} \), where \( h \) is the porous layer thickness, and \( K_p \) is the undeformed Darcy permeability. The study significantly improves our understanding of the dynamic response of soft porous media under rapid compression, which has broad impact on the study of transient load bearing phenomenon in biological systems and industry applications.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-H / 269

On the Reuse of Multiscale Basis Functions for the Approximation of Time-dependent Problems

Felipe Pereira\(^1\); Fabrício Sousa\(^2\); Het Mankad\(^3\)

\(^1\) The University of Texas at Dallas
\(^2\) University of Sao Paulo
\(^3\) The University of Texas at Dallas

Corresponding Author(s): luisfelipe.pereira@utdallas.edu

In the formulation of multiscale methods for second order elliptic equations that are based on domain decomposition procedures, (see e.g. the Multiscale Mortar Mixed Finite Element Method (MMMFEM) [1], the Multiscale Mixed Method (MuMM) [2], Multiscale Robin Coupled (MRC) [3], the Multiscale Hybrid - Mixed Finite Element Method (MHM) [4]) typically the computational domain is decomposed into subdomains, and for each subdomain a set of multiscale basis functions is numerically constructed. Consider the application of such a method to solve a multiphase flow problem [5] or in a Markov chain Monte Carlo (MCMC) uncertainty quantification study with a random walk sampler [6]. In these problems (from a time step to the next, for the flow problem and from one sample to the next, for the MCMC study) in principle, the multiscale basis functions should be recomputed because the coefficients of the underlying PDE will change. However, these changes are typically small. Thus, instead of calculating again all the multiscale basis function, we investigate the possibility of finding an approximate solution for the equation with modified coefficients using simple perturbation theory, followed by a downscaling step (needed to recover fine grid velocity fields for transport calculations). In this presentation, we focus on the MuMM [2], and we show that, in fact, the perturbation theory may produce accurate solutions, while taking advantage of multiscale basis function associated with the elliptic equation with distinct coefficients.

An efficient parallel algorithm is implemented in multi-core machines. Numerical experiments, where the perturbation theory results are compared with direct fine grid solutions, are presented and discussed.
References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 4-B / 148

On the macroscopic momentum balance equation for the fluid-fluid interfaces in two-phase porous media flows

Michele Starnoni\(^1\); Dubravka Pokrajac

\(^1\) University of Bergen

Corresponding Author(s): michele.starnoni@uib.no

Although two-phase flow in porous media is an established research field since decades, its theoretical background is still incomplete. In particular, while a universal definition of capillary pressure exists at the micro-scale, its upscaling to the macro-scale is still rather vague and a rigorous theory of capillarity at the macro-scale is missing. In this work, a new macroscopic theory of capillarity based on the volume averaging method is presented. The novel feature of the proposed averaging approach is the use of the superficial surface average for upscaling the relevant conservation equations for a surface. This allows for rigorous derivation of the macroscopic momentum balance equation for all the fluid-fluid interfaces contained within the Representative Elementary Volume (REV), thus resolving most of the shortcomings of previous studies, such as the averaging-scale inconsistency and the accounting for the different orientation of interfaces within the averaging volume. This latter aspect is described by an additional parameter arising in the proposed derivation, namely the intrinsic surface average of interface normal vectors \( \langle \mathbf{b}_n \rangle^{int} \). Furthermore, defining the macroscopic capillary pressure as the difference between the intrinsic surface averages of the bulk pressures, it is shown how the capillary pressure-fluid phase saturation curve can be determined in a more consistent manner by upscaling results of pore-scale simulations as oppose to traditional coreflooding experiments. This sets new challenges and opportunities for modelling unsaturated porous materials.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-C / 983

On using 3D-print technology to improve permanent cement plugs for P&A operations
Pierre Cerasi

1 SINTEF

Corresponding Author(s): pierre.cerasi@sintef.no

Setting a formation to formation cement plug in a well needing to be abandoned is a necessity, and the number of wells where this operation will have to be carried out increases each year in the North Sea. Paradoxically, where the mechanical and hydraulic integrity of this barrier matters most is also where these plugs are potentially weakest with today’s placement methods. This is in the shallower parts of the well to be plugged, serving as the last barrier for hindering a leakage to sensitive layers near the sea bottom. These plugs tend to vary in cement strength and stiffness, both radially out and from top to bottom. This is due to the feeble confinement and restricted spacer fluid density use at shallow depths, combined with potential damage during scraping of top of plug for verification of set cement.

This talk will outline the benefits of adopting rapidly evolving technology from 3D printing of materials and in particular concrete in the building industry. The potential advantages of this technology are:
- Constructing the plug layer by layer with identical properties for each layer
- Remove the need for spacer fluid flushes, since only small volumes will be cemented in each layer
- Continually controlling the compressive stress at which each plug layer is setting
- Perfect plug dimensions and geometry can be pre-programmed
- Hydration time, conditions and temperature can be controlled continually at the local scale.

Cost reductions can be envisaged by certifying quality and reproducibility of such printed cement plugs, thus removing the need for lengthy plug and reducing the redundancy in the number of required plugs.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 399

One-Dimensional Transient Inter-Porosity Flow Model in Tight Porous Media with Consideration of Fracture Pressure Depletion

Author(s): Shan Huang

Co-author(s): Yuedong Yao 1; Jing Wang

1 China University of Petroleum-Beijing

Corresponding Author(s): cuphbs@163.com

Tight porous media have the characteristics of extremely low permeability and the permeability of it is sensitive to the effective stress. Stimulated reservoir volume (SRV) is usually performed to improve the production of well in tight porous media. The SRV zone is usually considered as a dual-porosity medium in well test or numerical simulation due to the computationally efficient. The shape factor is the key of the dual-porosity model, which determines the ability of mass transfer between the matrix block and fracture. However, the conventional shape factor model which is usually obtained based on the assumptions of pseudo-steady state and constant fracture pressure, which lead to a poor application in the characterization of mass transfer between matrix and fracture in tight porous media.

In this paper, a new model was established by considering the effect of stress sensitivity and time-dependent fracture pressure boundary condition. Pedrosa substitution and perturbation method were applied to eliminate the nonlinearity of the model. By using the Laplace transformation method, the analytical solution in the Laplace domain was obtained. According to the Duhamel principle, the solution for time-dependent fracture pressure boundary condition was obtained. Then validation was performed to show that the model is valid. Finally, influence of stress-sensitivity and fracture
pressure depletion on shape factor and inter-porosity rate were discussed. Study shows that: Stress sensitivity of the matrix has an obvious influence on the inter-porosity flow. As the value of stress sensitivity coefficient increases, the value of the shape factor and inter-porosity rate decrease. After considering the impact of fracture pressure depletion, the effect of stress sensitivity on the shape factor is more significant. The faster the decreasing rate of fracture pressure, the larger the value of the shape factor at the initial time. However, the value of the shape factor is smaller at the later time due to the earlier and faster decreasing of fracture pressure. The inter-porosity rate will rise first to reach equilibrium and then decrease when the decreasing rate of fracture pressure is small. The new model can be used in the study of well test interpretation and numerical simulation, which provides a theoretical guidance for the reasonable development of tight porous media.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-H / 771

One-dimensional modeling, data assimilation and parameter estimation during nonlinear consolidation in randomly heterogeneous highly compressible aquitards

Berenice Zapata-Noberto1 ; Eric Morales-Casique2 ; Graciela del Socorro Herrera3

1 Posgrado en Ciencias de la Tierra, UNAM
2 Instituto de Geología, Universidad Nacional Autónoma de México
3 Universidad Nacional Autónoma de México

Corresponding Author(s): ericmc@geologia.unam.mx

The highly compressible nature of some aquitards leads to nonlinear consolidation where the groundwater flow parameters are stress-dependent. The case is further complicated by the heterogeneity of the hydrogeologic and geotechnical properties of the aquitards. To adequately model land subsidence in these systems, we develop a modeling approach to couple a nonlinear 1-D groundwater flow and consolidation model with a data assimilation scheme based on ensemble Kalman filter. This modeling approach allows to estimate the ensemble mean distribution of state variables and stress-dependent parameters, such as hydraulic conductivity (K), pore-pressure and total settlement. Zapata-Noberto et al. (2017) have shown that in randomly heterogeneous highly compressible aquitards under 1-D vertical flow, the parameter with largest impact on ensemble total settlement and its variance is K. We therefore consider the case where only K is randomly heterogeneous. We consider cases where pore-pressure and/or K measurements are available at given time intervals. We test our approach by solving the nonlinear flow and consolidation problem on a generated 1-D realization of lnK with exponential spatial correlation. These results are taken as our "true" solution. We take pore-pressure and/or lnK measurements” at different times from this “true” solution. The ensemble Kalman filter method is then employed to estimate ensemble mean distribution of lnK, pore-pressure and total settlement based on the sequential assimilation of those measurements. The ensemble-mean estimates from this procedure closely approximate those from the "true" solution. This procedure can be easily extended to other random variables such as compression index and void ratio.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-B / 848
Optimal non-woven filter media using multiscale simulations

M. Bruna¹ ; I.M. Griffiths² ; T. Grimble³ ; B. Hovell¹ ; G. Morris³ ; G. Printsypar²

¹ University of Oxford
² University of Oxford
³ Dyson Ltd.

Corresponding Author(s): galina.printsypar@maths.ox.ac.uk

Filtration of contaminants out of air is vital for many industrial applications. In particular, we are interested in the technology of air filtration used in vacuum cleaners produced by Dyson Ltd. In this study, we focus on predicting and improving the efficiency of the filter media used in vacuum cleaners. Filter media are usually characterized by different criteria. The first one is energy consumption. The small pressure drop or large permeability of filter media ensures economic use of energy. The second criterion is how efficient the filter media is at trapping the contaminants. The third criterion that we consider in this study is the dirt holding capacity, which characterizes how much contaminants the filter media can store over time and, therefore, how long it can be used. Using a multiscale model for filter efficiency simulations, we perform a parametric study to determine the characteristics of the filter medium with the best performance based on these criteria. The advantage of the multiscale method is that the coupled micro- and macroscale behaviour is captured without the computational expense of globally resolving the microscale filtration problem. We account for: single-phase fluid flow through the filter medium, contaminant transport with convection, diffusion and adsorption and the evolution of the filter medium microstructure due to the contaminant adsorption. We begin by comparing two given filter media to understand the differences in their behaviour. Then, we focus on the optimization of filter media by investigating the parameter space of different media characteristics, for example, porosity and fibre diameter.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-B / 634

Optimizing field-scale MICP with multi-scale micro-continuum OpenFOAM modeling

James Minto¹ ; Grainne El Mountassir² ; Rebecca Lunn³

¹ University of Strathclyde
² University of Strathclyde, Glasgow, United Kingdom

Corresponding Author(s): james.minto@strath.ac.uk

Microbially Induced Carbonate Precipitation (MICP) through the urea hydrolysis reaction has been extensively studied in the lab and implemented at field-scale several times, most notably for fracture sealing (Cuthbert et al., 2013; Phillips et al., 2016), for erosion control (Gomez et al., 2015), and for ground improvement (van Paassen et al., 2010). Grouting strategies used in industry are commonly based on experience derived from the injection of Ordinary Portland Cement, (e.g. use of the split-spacing method). Field-scale injection strategies for MICP are likely to differ considerably from traditional cement grout injections as:

i. the low viscosity of the injection fluids allows near-surface grouting with minimal risk of ground heave and the potential for larger soil/rock volumes to be treated around each injection point,
ii. strength improvement occurs without complete permeability reduction and multiple injections are required to incrementally reach the desired strength and permeability,
iii. flow velocity (to control bacteria attachment), pH adjustment (to control CaCO3 saturation state), and temperature (to control the rate of ureolysis) may all be used to limit blocking of the injection
points, and
iv. abstraction boreholes may be required for the removal of waste ammonium.

We present here a multi-scale micro-continuum MICP model implemented in OpenFOAM and solving fluid flow with the Navier-Stokes equations. The model is intended to inform the choice of injection strategy used in field-scale pilot projects and solves for 1) bacteria injection, velocity dependent attachment, and encapsulation within precipitating CaCO3; 2) re-agent transport, urea hydrolysis and CO3 production with Michaelis-Menten kinetics and 3) CaCO3 precipitation, porosity reduction, and subsequent flow path alteration.

In this model injections can be driven by a constant flow rate, constant pressure, or stepped flow rate and can be planar flow (e.g. for groundwater movement) as well as radial flow from/ to multiple injection/ abstraction wells. The model includes the ability to import 2D and 3D data from image analysis software ImageJ allowing X-ray micro-CT results from lab scale experiments to be modeled (at pore or micro-continuum scale) for validation purposes, and for heterogeneous site conditions to be modelled (at continuum-scale). A parametric sweep function is included to assess sensitivity to the choice of parameter values.

Results show that grouting with MICP is fundamentally different to grouting with cement. Operators may wish to replace sequential injection through a series of boreholes with simultaneous injection through multiple boreholes, or use abstraction boreholes to both collect waste ammonium and direct the transport of MICP re-agents.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-B / 551

Origin of sorption hysteresis of micro-porous polymers: an explanation based on hydrogen bonds

Author(s): Mingyang Chen

Co-author(s): Benoît Cosneau; Robert Guyer; Dominique Derome; Jan Carmeliet

1 ETH Zurich
2 CNRS/University Grenoble Alpes
3 UNR, LANL
4 Empa

Corresponding Author(s): minchen@ethz.ch

Soft nanoporous matter encompasses man-made materials such as compliant porous solids, intrinsically porous polymers and organic membranes as well as natural materials such as wood, bamboo, cotton and other plant-derived materials. These materials can undergo significant deformation during water adsorption because of strong coupling between the adsorption and mechanical properties. In addition, hysteresis is observed in the sorption isotherms of these materials. We find that sorption-induced deformation is the cause of hysteresis and analyze the special role played by the different types of hydrogen bonds.

We prepare three samples of amorphous cellulose as the host material considering its wide presence
in nature. Water sorption and deformation are simulated with a hybrid Grand Canonical ensemble (GCMC)/Molecular Dynamics (MD) method. The sorption isotherms simulated for each of the three samples exhibit significant hysteresis and the simulation results agree well with experimental data on low-crystalline cellulose. Significant hysteresis is observed as also seen in a variety of micro-porous polymers. The volumetric strain is monitored and shows significant swelling strains reaching as high as 36% at the saturation point. We note that, if we eliminate the deforming effect by freezing the cellulose at the dry state or the saturated state and then conduct an additional adsorption or desorption loop, the simulated isotherms significantly deviate from the experiments and the hysteresis disappears. This shows that the hysteretic sorption strongly depends on the deformation of the system.

We explore the mechanism of sorption hysteresis by further interrogating the systems. As amorphous cellulose is a non-cross-linked polymer, hydrogen bonds play a crucial role in both sorption and deformation processes. Hydrogen bonds are analyzed to monitor the interactions inside the system, revealing different configurations during adsorption and desorption. We find that the origin of sorption hysteresis in amorphous cellulose can be attributed to the process of creation of new adsorption sites due to hydrogen bond breaking during swelling. During adsorption process, some cellulose-to-cellulose hydrogen bonds (HBCC) change into cellulose-to-water hydrogen bonds (HBCW). However, the recovery of these new adsorption sites back to HBCC during desorption is less likely since they more likely remain occupied by water molecules. Consequently, the system accommodates the same amount of water molecules distributed over more sorption sites at lower energy state during desorption process, leading to hysteresis in the sorption isotherms observed in both experiments and simulations. Moreover, sorption hysteresis is also shown to have a significant influence on other important properties such as pore size distribution and bulk modulus.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 944

Overview of Experimental Systems and Approaches Supporting In Situ Mineral Precipitation Research

Adrienne Phillips¹ ; Robin Gerlach¹ ; Joe Eldring¹ ; Randy Hiebert² ; Al Cunningham³

¹ Montana State University
² Montana Emergent Technology
³ Center for Biofilm Engineering, Montana State University

Corresponding Author(s): adrienne.phillips@montana.edu

The Center for Biofilm Engineering (CBE) at Montana State University has a long, successful history of investigating biofilm and mineral precipitation processes in subsurface environments. This poster summarizes many of the experimental approaches the CBE has taken to develop field-suitable technologies. There are numerous applications for engineered biomineralization. The CBE has largely focused on the sealing of leakage pathways, water remediation, soil stabilization, dust suppression and enhanced resource recovery. The experimental systems to examine these engineering applications have been designed to interrogate biofilm and mineral precipitation processes in a variety of environments, conditions, geometries and chemistries. This poster will highlight experimental systems from low pressure to high pressure, bench scale to field scale and low temperature to high temperature.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 3-H / 633

POROUS MEDIA INVESTIGATION USING DUAL NETWORK MODELS

Zohaib Atiq Khan1; Jeff Thomas Gostick2

1 University of Waterloo, ON, Canada
2 University of Waterloo

Corresponding Author(s): zatiqkha@uwaterloo.ca

Extracting structural information, such as pore networks, from tomographic images is a powerful tool for the study of porous materials. Pore network models are used for predicting different physical properties such as permeability and tortuosity, and simulating chemical process such as reactive transport. Due to its inherent simplifications, pore network modelling requires far less computation cost and time as compared to other pore-scale modelling approaches like lattice Boltzmann and finite volume method allowing researchers to investigate larger volume of porous materials[1,2]. Consequently, they are being increasingly used to study multiphysics in various devices where the porous structure plays a critical role in performance[3], but true pore-scale modeling is computationally infeasible.

In traditional pore network modelling applications, the solid phase network is not usually considered since the only the fluid phase is of interest. In electrochemical devices, however, electron and heat transport through the solid phase of the electrode are equally important. In this work, we report on the concept of extracting dual network models from tomographic images, that includes information for both solid and pore phases and interlinking of these phases with each other. These dual network models provide a new avenue for understanding many critical chemical process like reaction-diffusion in catalysts as well as batteries charging and discharging kinetics in porous electrodes, both of which require understanding the solid phase transport.

The presented algorithm is based on an algorithm recently published by our group[3], and produces output that is compatible with the open-source modeling package OpenPNM[4].

References:

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 1096

PVDF hollow fiber membranes with different morphologies in direct-contact membrane distillation

Li Yue1; Peng Yuelian2

Corresponding Author(s): pyl@bjut.edu.cn
In this study, polyvinylidene fluoride (PVDF) hollow fibers with different morphologies have been fabricated via a dry-jet wet spinning process and tested for membrane distillation (MD). The effects of PVDF content and solvents, dimethylacetamide (DMAc) and triethylphosphate (TEP), on the morphology, pore structure geometry and MD performance were investigated. Phase separation mechanism of PVDF/additives/solvent systems was carefully studied via a phase diagram. Direct-contact membrane distillation (DCMD) for desalination was carried out to evaluate membrane permeability and salt rejection. A PVDF/polyethylene-glycol (PEG)/DMAc system produced a typical finger-sponge-finger-like structure in an instantaneous liquid-liquid (L-L) demixing, but an increase of PVDF content delayed the L-L phase separation, leading to a sponge-like cross-section. However, using TEP instead of DMAc, a bi-continuous morphology would be formed during crystallization. The hollow fibers fabricated from a PVDF/PEG/TEP system showed high permeability, long-term stability with big pores, high pore connectivity and narrow pore size distribution, potentially suitable for water and wastewater applications.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-D / 546

Parallel NMR cryoporometry, relaxometry and diffusimetry studies of porous carbon aerogels

Author(s): István Bányai

Co-author(s): Mónika Kéri; Dávid Nyul; Balázs Nagy; Krisztina László

1 University of Debrecen, Department of Physical Chemistry
2 University of Debrecen, Department of Physical Chemistry
3 Budapest University of Technology and Economics, Dept. of Physical Chemistry and Materials Science

Corresponding Author(s): banyai.istvan@science.unideb.hu

NMR cryoporometry, relaxometry and diffusimetry are widely used for the characterization of porous materials. In this work we investigated resorcinol-formaldehyde (RF) based carbon aerogels, prepared in different ways, with all the three NMR techniques parallel in aqueous medium. This made possible the comprehensive characterization of the aerogels concerning pore size and shape, pore volume, hydrophilic/hydrophobic properties, saturation mechanism.

T2 relaxation times and diffusion coefficients for water in the aerogels were determined at different water contents by low field 1H-NMR methodology. Cryoporometric measurements were carried out at several saturation states by high field 1H-NMR. The results show that the hydrophobic carbon aerogels contain hydrophilic sites, which bind the moisture of the air resulting in short T2 values. Spherical pores with 45 nm diameter get saturated at about 4 g/g water content according to the cryoporometry. First, pores get filled with water, and then the number of filled pores increases. At higher water contents cylindrical channels appear. From the cryoporometric results, combining with the low-field relaxometry, we could deduce the surface relaxation time and surface layer thickness of these materials. The mechanism of pore saturation was confirmed by NMR diffusimetry showing restricted diffusion due to the pore walls and diffusion through gas phase in partially filled samples.

Different ratios of water and ionic liquid were used during the preparation process of RF hydrogels. The different compositions of solvents changed the pore size and the hydrophilic/hydrophobic character of the prepared carbon aerogels. The characterization, beyond NMR, was also carried out by means of water and nitrogen adsorption methods. The comparative analysis of the adsorption and NMR techniques could give a detailed picture for the morphology of the carbon aerogels, the effect of preparation medium and the mechanism of water loading.

References:

Parallel implementation of a multiscale mixed finite method for waterflood displacement in five-spot patterns

Felipe Pereira¹ ; Eduardo Abreu² ; Joel Moraes³ ; Luis Santos³ ; Paola Ferraz⁴

¹ Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA
² University of Campinas, Sao Paulo, Brazil
³ University of Campinas - SP - Brazil
⁴ University of Campinas - Sao Paulo - Brazil

Corresponding Author(s): eabreu@ime.unicamp.br

In this work, we have performed an efficient implementation of the multiscale mixed method MuMM introduced in [1], that is based on a non-overlapping iterative domain decomposition procedure with novel Robin interface conditions (see also [2] where the variational formulation of [1] was presented). We also performed a numerical study to built multiscale mixed basis functions to find an optimum set of mesh grid parameters defined in the subdomains associated with the coarsest scale to a sensitivity analysis aiming a better selection of optimum development scenarios for waterflood displacement in five-spot patterns. The reserve growth potential of existing conventional oil reservoirs world-wide is huge and set to continue, in despite from other emerging energy resources. Locally conservative hybridized mixed finite elements are used for the spatial discretization of the underlying 3D Elliptic problem linked to the quarter five-spot Darcy flow at hand. This procedure can be used to be effective for practical purposes on the development scenarios for waterflood displacement in a five-spot pattern. The procedure fits well in heterogeneous processing units (CPU-GPU), along with Message Passing Interface technology for clusters. This work aims to produce a simple, fast and efficient numerical tool to evaluate selection of optimum number of wells and their possible optimum location to prevent the wastage of capital investment and for improving waterflooding recovery in oil reservoir engineering.


References:


Poster 1 / 1093

Parameter Identification in Confined Aquifers using a Predictor-Corrector Scheme of the Differential System Method

Liliana Guadalupe Salvador\textsuperscript{None} ; Miguel Ángel Moreles Vázquez\textsuperscript{None}

Corresponding Author(s): liligs@cimat.mx

The inverse problem of parameter identification consists in the optimal determination of model parameters using water-level observations. We are concerned with the estimation of the transmissivity and storativity in a confined aquifer in transient conditions. One of the approach used to solve this problem, is called the Differential System (DS) method. It is based on the solution of a Cauchy problem. Because of the numerical derivatives need to be calculated, the issue with this method is when noisy data are used. In this work, we propose an improvement to the DS method by using a predictor-corrector scheme. For the predictor part, we consider an estimator obtained from the Bayesian formulation problem. The study case presented here is a synthetic but realistic aquifer; the model was chosen in order to check how the estimation is made in complicated conditions.

References:


Click here to agree

Parallel 2-H / 1000

Parameter estimation and steady-state groundwater flow prediction via three stochastic approaches

Abel F. Hernández\textsuperscript{1} ; Jessica V. Briseño\textsuperscript{2} ; Eric Morales-Casique\textsuperscript{2} ; Graciela S. Herrera\textsuperscript{3} ; Oscar Escolero-Fuentes\textsuperscript{2}

\[1\] Gerencia de Geotermia, Instituto Nacional de Electricidad y Energías Limpias, Cuernavaca, Mor. C.P. 62490, México.

\[2\] Instituto de Geología, Universidad Nacional Autónoma de México, México, D.F. C.P. 04510, México

\[3\] Instituto de Geofísica, Universidad Nacional Autónoma de México, México, D.F. C.P. 04510, México

Corresponding Author(s):

We consider log hydraulic conductivity (Y) as uncertain and predict steady-state groundwater head (h) through three different, independent approaches. The first two of them are based on the ensemble Kalman filter (EnKF), their difference being in the way statistical moments (SM) of state variables and parameters are estimated numerically before the Kalman filter is applied. Whereas in the first approach Monte Carlo simulations are used for this aim, in the second approach the required SM are obtained by solving nonlocal stochastic moment equations (ME) of steady state flow. In the third approach, the ME are subjected to a geostatistical stochastic inversion using a pilot point parameterization. Additionally, a less computationally demanding version for each of the first two approaches was obtained by modifying its algorithm to estimate Y geostatistically (i.e., using generalized kriging) at the pilot points of the third method instead of estimating over the entire grid as its original algorithm does. The three methods and their second versions were applied separately in a synthetic 2D steady-state groundwater flow domain to compare their performances. Our results show that all methods and associated versions were effective in estimating h, reaching at least 81%
of predictive coverage. For log hydraulic conductivity similar accuracies were obtained in terms of the mean absolute value error for all methods. In terms of numerical performance, we found that coupling the EnKF methods with kriging reduces the CPU time required for data assimilation while both estimation accuracy and uncertainty do not deteriorate significantly.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-D / 304

Particle size distribution match optimization by a superposition method for artificial core synthesis

Joseph Fu1 ; Xiang'an Yue2 ; Bo Zhang2

1 China University of Petroleum (Beijing)
2 China University of Petroleum (Beijing)

Corresponding Author(s): josephfu100@yahoo.com

Enhanced oil recovery testing often relies on either a sand pack filled with sand or use Berea sandstone that doesn’t take into account the full range of petrophysical properties of the actual reservoir. Among the most important reservoir petrophysical properties are the particle sizes and their distribution that serves as the key parameter that influences strongly other key petrophysical parameters such as permeability, porosity, pore throat distribution, capillary pressure, etc. In this work, the authors have devised a new method to synthesize an artificial core in which the porosity, permeability, and particle size distribution nearly match that of a target natural reservoir core: 1. The method entails having the thin section prepared on a sliced target natural reservoir core. 2. The particle size distribution analysis is done on the slice under a microscope. 3. Different sizes of sieved sands have particle size distribution analysis done by a laser particle size analyzer. 4. The particle size analysis of the sands and the target natural reservoir core is superimposed on the same plot and the best-fitting sand is visually picked out. 5. The best-fitting mesh size is either used directly or sieved to cut off a smaller or bigger fraction not found in the particle size distribution of the target natural reservoir core. 6. The sieved sands are compressed into an artificial core with addition of other micron sized sands served as fillers with a specialized adhesive at a set compression time and pressure. 7. The synthesized artificial core is sent for porosity and permeability analysis. 8. If porosity and permeability is not within 5% and 10% of the target respectively, then more fine sand fillers are used to dial down the porosity and permeability on another attempt to synthesizing another core. 9. If porosity and permeability are both matched within acceptable error, the artificial core is sent for thin section particle size distribution analysis. 10. If the medium size of the artificial core’s particle size distribution and the shape of the distribution doesn’t match the target, then another adjustment is made on the sand size and the process is repeated until it does. Through several trial and error attempts using this method, the particle size distribution, permeability, and porosity of the artificial core is closely matched to a set target natural reservoir core. Using this method, a more robust artificial core can be synthesized for use in enhance oil recovery testing.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 568

Pattern Formation and Mixing Dynamics in Three-Dimensional Non-Boussinesq Solutal Convection
Amin Amooie¹ ; Mohamad Reza Soltanian² ; Joachim Moortgat³

¹ The Ohio State University
² University of Cincinnati

Corresponding Author(s): amooie.1@osu.edu

Motivated by the process of convective mixing in porous media, here we study the pattern-formation and coarsening dynamics arising from dissolution of CO₂ in a single-aqueous phase during three-dimensional (3D) Rayleigh-Bénard-Darcy convection. Our focus is on comparing the pattern-formation aspects of solutal convection between conditions of constant concentration and constant flux prescribed at top boundary. In the constant-flux case, a low (constant) injection-rate of CO₂ is considered, such that all CO₂ dissolves and the system remains indefinitely in single phase. We adopt non-Boussinesq, compressible formulation, whereby the nonlinear phase behavior and density variation of mixture as a function of pressure, temperature, and solute concentration are fully accounted for. We perform high-resolution finite element simulations of 3D convective mixing to examine the interplay between the density-driven hydrodynamic instability and the pattern formation at top boundary as well as various cross sections. We find that gravitational instabilities—triggered at the boundary layer by the local increase in density following CO₂ dissolution—further develop into columnar plumes of CO₂-rich brine because of self-organization of concentration field in the diffusive boundary layer as a cellular network structure irrespective of top boundary type. While such pattern formation occurs at top boundary for the constant-flux case, it can be captured only below the top boundary for the constant-concentration case. By studying the statistics of the cellular network and concentration field, we identify various regimes of finger coarsening over time for both model types, and show the existence of a quasi-steady state where the average cell size at top boundary, or below top for the constant-concentration case, remains constant due to an equilibrium between cell division and merging in correlation with a constant-mixing rate regime. The morphology of mixing patterns in three dimensions for different types of boundary conditions has implications to numerous density-driven problems in fluid mechanics as well as in environmental and geological settings.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 117

Percolation Behavior in Catalytic Porous Materials

Author(s): Karrar Alofarain

Co-author(s): Sofyane Abbou ; Ezequiel Medici ; Kazuya Tajiri ; Jeffrey Allen

Corresponding Author(s): ktalofar@mtu.edu

Liquid water is produced during hydrogen-oxygen reactions in proton exchange membrane fuel cells, which operate at temperatures below 100 C. Proper water management is important to achieve high performance and durability. The behavior of liquid water percolating through the catalyst layer of PEM fuel cells is not understood, and has not be experimentally characterized. This is in part due to the complex structure of the catalyst layer that includes catalyst support (typically carbon) for electron and thermal transport, catalyst (typically Pt), ionomer for protonic transport, and a pore space for reactant and water transport. The ionomer provides additional complexity in that it swells as water is absorbed. In order to characterize the relationship between catalyst layer structure and morphology with liquid water percolation, a pseudo-Hele-Shaw test has been developed in which a liquid is injected into a catalyst layer. The liquid displaced air to generate imbibition or drainage flows depending upon wettability of the catalyst layer. Variations in environmental humidity affect ionomer with swelling occurring at high relative humidities. Ionomer swelling causes a shift in the pore size distribution with a subsequent increase in injection pressure during percolation testing. To isolate the effect of active participation by the catalyst layer, two liquids are used during testing. The first is a fluorinert that does not interact with the ionomer and the second is water.
Parallel 8-A / 749

Permeability Reduction Caused by Multiple Treatments of Biomineral Precipitation in Homogeneous Porous Media: Experimental Study and Pore Scale Modelling

Daehyun Kim¹; Nariman Mahabadi¹; Jaewon Jang²; Leon van Paassen¹

¹ Arizona State University
² Hanyang University

Corresponding Author(s): dkim147@asu.edu

Several biochemical processes have been investigated to modify engineering properties of soil. Biomineral precipitation can increase strength and stiffness, and reduce porosity and permeability. Enzymatically induced calcium carbonate precipitation (EICP) is a biochemical process in which urea is hydrolyzed into ammonium and inorganic carbon, which promotes carbonate mineral precipitation. Different morphologies and patterns of carbonate mineral precipitation, such as particle surface coating, pore filling, and soil particle contact bonding have been observed in the previous studies, in which the mineral structure and distribution has been evaluated after the completion of the treatment using SEM (Scanning Electron Microscope) imaging and XRD (X-ray Diffractometer) structural analysis. As the hydro-mechanical properties of soils can be significantly affected by the distribution of precipitated mineral in the pore space it is important to investigate these properties at pore scale. In this research, an EICP reaction medium is injected into a microfluidic channel to observe the entire process of carbonate mineral precipitation through several cycles of EICP treatment in the porous medium. Mineral phase changes and concomitant porosity and permeability reduction throughout the system are evaluated by image processing. A two-dimensional simulation model involving urea hydrolysis and mineral precipitation is developed, and the results are analyzed in comparison to the experimental results.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-F / 480

Permeability evolution of thermo-mechanically coupled granite

Zijun FengNone; Yangsheng ZhaoNone

Corresponding Author(s):

Permeability of Luhui granite with 200mm in diameter and 400mm long was measured at triaxial stresses and elevated temperature using 600°C20MN servo-controlled triaxial rock mechanics testing machine. It is found that 300°C is the threshold temperature (Tc) of permeability change with temperature in thermally cracked granite. The magnitude of permeability is 10-7D with a low increase below Tc and the permeability whose magnitude is 10-6D increases drastically with high amplitude at 300°C-400°C while the magnitude is 10-5D at 400°C. Simultaneously, the change of micro-crack quantity in thermally cracked Luhui granite at temperature up to 400°C was quantificationally investigated by MPV micro-photometer. Two peaks of micro-crack quantity that the length is more than 5µm and 10µm respectively exist at temperature up to 400°C. The temperature scope where
micro-crack quantity peak appears in length>5µm is less than that in length>10µm. The quantity of micro-crack whose length is more than 10µm increases sharply at the rate of one per ten centigrade at temperature above 300°C. The drastic increase of micro crack above 300°C is the main reason that permeability increases sharply at temperature above 300°C in thermally cracked granite. Compared with preheated results, thermal and mechanical coupled effect can more heavily affect granite permeability than only thermal effect.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 533

Petrographic characterization of low-permeable to tight turbidite sandstone from Eocene Shahejie Formation using micro-CT.

Muhammad Jawad Munawar1; Veerle Cnudde2; Chengyan Lin1; Tom Bultreys1; Chunmei Dong1; Zhang Xianguo1; Wesley Deboever2,3; Muhammad Aleem Zahir4; Yuqi Wu4

1 China University of Petroleum (East China)
2 Department of Geology, PProGReSS/UGCT, Ghent University,
3 China University of Petroleum (East China)
4 Imperial College London

Corresponding Author(s):

Pore scale flow simulations in reservoir rocks heavily depend on characterizing and modeling of the pore space. Single scale and multiscale pore network extraction from micro-CT images are going through extensive development. However, the choice of pore network extractions method is sensitive to the rock nature (homogenous, complex or microporous). Additionally, the success of the pore network to predict flow properties relies on image quality and image segmentation. In this study, we characterized four samples from a low permeable to tight sandstone reservoir using micro-CT at the expertise Centre for X-ray Tomography at Ghent University (www.ugct.ugent.be) to assess the impact of microporosity on the rock model. All samples were scanned at a resolution of 1.5 to 1.7 micron. As the samples can be categorized as illite rich and kaolinite rich, attention towards the clay minerals were given as they play a vital role to influence microporosity. ( pore size < 1.7 micron) Image segmentation analysis from micro-CT images indicated that 5-6 % of microporous regions were present in kaolinite rich sandstone, while illite rich sandstone displayed 1.7-1.8 % microporous regions. Correlation of mineral phase data from micro-CT and XRD revealed that the microporosity consisted mainly out of dissolved feldspar grains and clay mixed cement. In kaolinite rich, macropore system does not percolate without micro pores, while in illite rich sandstone the pore system percolates without micro pores. In illite rich sandstone, the total MICP porosity is equal to the macroporosity (pore diameter >1.7 micron) determined on the 3D micro-CT, this means that the macropores are well connected and micro pores do not play any role in the flow process. However, in kaolinite rich sandstone, the macroporosity determined from the 3D X-ray micro-CT images is far less (almost 50 %) than the total MICP porosity which means that almost 50 % of the porosity consisted out of pores that were not detected by the micro-CT scan. In these kinds of rocks, the pore system does not percolate without the micro pores and a multiscale approach is needed to characterize such complex rock.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-A / 696
Phase Equilibria in CO2-Multicomponent Hydrocarbon Systems in Shale Organic Nanopores: A Coarse Grained Molecular Simulation Study

Ali Takbiri-Borujeni\textsuperscript{1} ; Mohammad Kazemi\textsuperscript{2}

\textsuperscript{1} West Virginia University
\textsuperscript{2} Kansas University

Corresponding Author(s): altakhiri@mail.wvu.edu

Studying the phase behavior of complex hydrocarbon and hydrocarbon/CO\textsubscript{2} mixtures in kerogen structures is extremely important for understanding the mechanisms involved in enhanced gas recovery, storage, and production of hydrocarbons from shale. The objective of this work is to determine the phase behavior of a number of binary, ternary, and multicomponent CO\textsubscript{2}/hydrocarbon systems using molecular dynamics simulation in three dimensional kerogen structure of type IIA. These systems include CO\textsubscript{2}/n-Hexadecane, CO\textsubscript{2}/n-Eicosane, CO\textsubscript{2}/n-Butane/n-Decane, and CO\textsubscript{2}/synthetic oil. The kerogen molecule is prepared based on detailed structural analysis of NMR experiments. In order to build a representative solid state model of kerogen, eight kerogen molecules are placed in a periodic cubic cell. Once the initial configuration of kerogen molecules is prepared, constant-temperature constant-volume (NVT) simulations and then constant-temperature constant-pressure (NPT) simulations are performed to obtain the final structure. The SAFT-\(\gamma\) coarse graining methodology is used to develop force fields for the fluid-phase behavior of hydrocarbon/CO\textsubscript{2} mixtures comprising CO\textsubscript{2} and \(n\)-alkanes. The densities, phase compositions, and volume of each phase in kerogen are determined at different overall compositions and pressures and compared with unconfined case. For the final kerogen structure, density values are calculated and compared with the reported density range for kerogen density. A good agreement is found between the experimental densities and our kerogen molecular structure density. Calculated phase equilibria for the unconfined system (where experimental measurements are available) are in fair agreement with experimental data. The liquid phase density did not change significantly in confined case (in kerogen) compared with that of unconfined (or bulk). However, the heavier components tend to vaporize in kerogen structure compared with the unconfined case. For example, \(n\)-decane have much higher composition in vapor phase in kerogen compared to bulk condition. Furthermore, as the pore diameter increases, the phase envelopes approach the bulk conditions.

Experimental measurements of the phase behavior of hydrocarbon mixtures in confined systems are extremely difficult, if not impossible, with current technologies. This work is one of the few in-depth investigations of the phase behavior in organic matters of shale. The results of this study can potentially modify the equation of state for shale reservoirs and help in understanding the transport mechanism in nanoscale pores.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-A / 62

Phase field formulations for reactive two-phase flow

Author(s): Carina Bringedal\textsuperscript{1}

Co-author(s): Sorin Pop \textsuperscript{1}

\textsuperscript{1} Hasselt University

Corresponding Author(s): carina.bringedal@uhasselt.be

Two-phase flow problems and reactive flow with changing pore geometry both include a free boundary at the pore scale. Chemical reactions as mineral precipitation and dissolution can alter the pore structure; hence the fluid-grain interface evolves following the reaction rates. The presence of two
immiscible fluids introduces an evolving fluid-fluid interface depending on the flow itself and surface tension. Problems with evolving boundaries are usually formulated through the location of the sharp interfaces, but we here propose phase field formulations that allow formulating the relevant processes on a larger regular domain with the evolving interface appearing as a diffuse transition of non-zero width. From a numerical point of view, the phase field formulation is simpler as the small-scale structures do not need to be explicitly resolved but is instead captured through the evolution of the phase fields. In the limit as the diffuse interface width approaches zero, the usual sharp interface formulation is obtained. Further, the pore scale phase field formulations can be upscaled to the macro (Darcy) scale using homogenization.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 580

Phase separation in capillary channel flow using porous media

Author(s): Kamal Singh Bisht
None

Co-author(s): Michael Dreyer

Corresponding Author(s): kamal.bisht@zarm.uni-bremen.de

Kamal S. Bisht, Michael E. Dreyer, University of Bremen, Faculty of Production Engineering, Department of Fluid Mechanics, ZARM, University of Bremen, Germany

In propellant management devices (PMD), porous media are widely used for the phase separation process and delivery of vapor free propellant. However, instability of the free surface flows in open capillary channels limits the flow rate capacity and affects the effectiveness of the porous media. In low-gravity conditions, capillary pressure only balances the pressure difference across the liquid-gas interface. At the critical flow rate, the maximum capillary pressure is exceeded; the free surface collapses and gas bubbles are ingested into the liquid. The presence of gas degrades the quality of the propellant and severely affects the engine efficiency. In this project, a setup with a metallic porous screen covering a rectangular groove channel is investigated to obtain a higher flow rate in capillary channels without collapse of the free surface. The saturated porous screen permits liquid to pass through but acts as a barrier to the gas breakthrough until the differential pressure across the screen exceeds to the bubble point pressure.

This feature is governed by porous media properties such as permeability, porosity, wettability and pore diameter. A theoretical study has been done and is currently under investigation using numerical tools and ground tests. The computations are performed with Matlab and the computational fluid dynamics program Ansys Fluent. The setup for the experimental test facility is defined which shall be tested next year in summer during drop tower test. The theoretical, experimental and numerical results will be presented in the talk.

References:


Click here to agree
Physical simulation experiment and numerical inversion of the full lifecycle development of shale gas well

Author(s): Liyou Ye
Co-author(s): Shusheng Gao, Huaxun Liu, Zhiming Hu, Wenqing Zhu

1 Department of Porous Flow & Fluid Mechanics, RIPED, PetroChina

Corresponding Author(s): yeliyou69@petrochina.com.cn

Shale reservoirs generally have very low porosity and permeability and complex occurrence and transport state, which lead to its unique L-curve production characteristics, representing complicated flow mechanism. A physical experiment using full diameter core was designed to simulate the full lifecycle development process of the shale gas well. From the experiment, many important and comprehensive production dates corresponding to the real production process, such as pressure and daily gas production, were obtained, which solves the difficulty to collect real production dates derived from short production time or operation discontinuity of the shale gas well. This experiment lasted 1631 days and the results showed that there is an ideal similarity of production between physical simulation and shale gas well. Based on the simulation data, the core’s critical desorption pressure(12MPa), the free gas volume(3820.8ml), and adsorbed gas volume(2152.2ml) were confirmed accurately. Furthermore, the ratio of free gas and adsorbed gas in daily gas production at different time and pressure, the lasting production time and final recovery efficiency at the abandonment pressure were accurately determined. Based on well test and similarity theory, numerical inversion was applied to calculate the production dynamic curve of shale gas well and predict the development effect of gas well based on the similarity between core and gas well.

References:

Acceptance of Terms and Conditions:
Click here to agree

Pore Network Stitching for Pore-to-Core Upscaling of Capillary-Dominated Two-Phase Flow in Heterogeneous Natural Reservoir Rocks

Amir Kohanpur, Albert Valocchi

1 University of Illinois at Urbana-Champaign
2 Univ Illinois

Corresponding Author(s): kohanpu2@illinois.edu

Physics of two-phase flows in heterogeneous natural rocks plays an important role in many applications, such as carbon sequestration in deep saline reservoirs and recovery of oil from hydrocarbon reservoirs. Although pore-scale models are used to compute macroscopic average properties required in field-scale simulators, most work is limited to small sample size. There is a need for pore-scale models that can accurately represent the 3D complex pore structure and heterogeneity of real media. Pore network modeling (PNM) simplifies the geometry and flow equations at pore-scale, but can provide characteristic curves in capillary-dominated systems on fairly large samples with huge saving on computational costs compare to direct numerical simulation methods. However, there are limitations for attaining a large representative pore network for heterogeneous cores such as technical limits on scanning size to discern void space and computational limits on pore network extraction methods. To address this issue, we propose a novel pore network stitching method to provide large-enough representative pore network for a core.
In this study, we use industrial (as core-scale) and micro-CT (as pore-scale) scans of actual reservoir rock samples to characterize the pore structure of a core. Few signature parts of the core are selected from industrial scans, and their micro-CT scans are taken. Equivalent 3D pore network of each signature part is extracted by applying maximal ball pore network extraction algorithm. The space between signature networks is filled by using stochastic random network generator that uses statistics (radius, shape factor, connection number, and length of pore elements) of all signature networks and a layered stitching method that glues network pieces. The outcome is a large pore network that can be used in a fast quasi-static PNM solver to obtain absolute permeability, relative permeability and capillary pressure curves. We have tested the developed method on various generated and extracted networks by 1D stitching direction, and it will be improved and extended to 2D and 3D stitching directions.

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

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-B / 772

Pore Scale Simulation of Biogenic Gas Formation and Migration in Porous Media

Nariman Mahabadi\textsuperscript{1} ; Leon van Paassen\textsuperscript{1}

\textsuperscript{1} Arizona State University

Corresponding Author(s): nmahabad@asu.edu

The biogenic gas behavior in porous media, which includes bubble nucleation and growth, migration, coalescence and trapping is affected by the gas generation rate, distribution of reactive sites and the pore scale characteristics of the sediment. In this study, experiments are performed using a micro-fluidic chip in which different gas bubble behavior mechanisms in the porous media are observed. Secondly, the behavior of biogenic gas is simulated using a pore-network model extracted from the 3D X-ray image of an in-situ sediment. The formation of biogenic gas bubbles is modeled using the classical gas nucleation theory. Several numerical algorithms and criteria developed for the expansion of gas bubbles during the biogenic gas formation, size-dependent rising velocity of gas bubbles, bubble coalescence, slug formation and movement, escaping, and trapping in the pore space. The amount of produced gas bubbles, residual gas saturation and hydraulic conductivity are calculated during the simulations. Results of the simulation are qualitatively compared with the microfluidic chip experiments.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 435

Pore Structure Evaluation and Fluid Assessment for Permian Carya-ginia Shale

Yujie Yuan\textsuperscript{1} ; Reza Rezaee\textsuperscript{1}
Pore network modelling of single phase flow in functionalized porous materials: permeability prediction and validation

Author(s): Agnese Piovesan¹

Co-author(s): Clement Achille ² ; Pieter Verboven ³ ; Rob Ameloot ⁴ ; Bart Nicolai ⁵

¹ KU Leuven – University of Leuven, Division BIOSYST-MeBioS
² 2 KU Leuven – University of Leuven, Center for Surface Chemistry and Catalysis
³ 1 KU Leuven – University of Leuven, Division BIOSYST-MeBioS
⁴ KU Leuven – University of Leuven, Center for Surface Chemistry and Catalysis
⁵ KU Leuven – University of Leuven, Division BIOSYST-MeBioS

Corresponding Author(s): agnese.piovesan@kuleuven.be

Capillarity driven lab-on-chips (LOC) are small cheap devices dedicated to perform diagnostics autonomously. To operate the chips, fluids flow in functionalized porous channels. Performance of the LOC however depends on the microporous fluid flow characteristics of the device. Pore-network (PN) models are a powerful tool to investigate transport phenomena at the pore scale while avoiding expensive and time consuming computational fluid dynamics (CFD) direct simulations. High resolution imaging techniques allow topologically representative PNs to be extracted on which fluid flow can be simulated. In this work, 1 μm resolution X-Ray computed tomography (CT) scans were executed on functionalized porous matrixes of poly-methyl methacrylate (PMMA). The reconstructed images were binarized to isolate the pore space. A watershed algorithm was applied to obtain divided pores as a basis for the material PN. The PN was composed by nodes representing the pores interconnected by channels with simplified geometry, representing the pores throats. Two different channels geometries were considered: cylindrical channels with the diameter computed as the average between pore and pore throat equivalent diameters, and bi-conical shaped channels. The latter were represented as stacks of 1 pixel thick cylinders with diameter varying smoothly from the pore to the pore throat.

The obtained PNs were employed to simulate single phase flow and compute the material permeability by means of the Darcy’s law and verified by measured values and CFD simulations. The effect of
different parameters on the obtained permeability was investigated. In particular, the study focused on the number of seeds used for the watershed algorithm, the channel geometry as well as the pore shape, that was taken into account through the sphericity parameter. 
A higher number of watershed seeds led to a more accurate solution, since a more precise porespace subdivision is generated, but to longer computational times as well. Cylindrical channels were found to produce permeability values around 250% higher than the bi-conical ones at the same number of seeds. As a result when cylindrical channels were used, a permeability value comparable to both the CFD and experimental ones was obtained with a number of seeds about five times higher with respect to bi-conical channels. Eventually, considering pore sphericity was proved to reduce permeability dependency on both the number of seeds and the channels geometry. When bi-conical channels were used and pore sphericity was taken into account, permeability values comparable to the CFD and experimental results were obtained with a number of seeds eight times smaller, than when cylindrical channels with no sphericity corrections were employed. This corresponded to a reduction of computational time of about 60%. The developed PN model, therefore, allows material permeability to be computed with good accuracy in significantly shorter time with respect not only to direct CFD, but also to other PN models (shape). In a next step, the main focus will be on the application of the extracted PN to study multi-phase capillary flow.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 1099

Pore scale modeling of acoustic events
Abhishek Agrawal\textsuperscript{None} ; Ahmad Sakhaee-pour\textsuperscript{1}

\textsuperscript{1} University of Houston

Corresponding Author(s): abhkagrawal@gmail.com

It is well established that acoustic emission is generated during hydraulic fracturing. Acoustic emission is used to find the volume effected by hydraulic fracturing, which is known as stimulated rock volume (SRV). Understanding the flow and transport properties of SRV is important as it effects the EUR of the oil reservoirs. In this study we analyze the change in permeability, an important transport property, using pore scale modeling of the acoustic events.

We conducted a hydraulic fracturing experiment on a block of sandstone in the lab and recorded the acoustic emission events generated during fracturing; the hypocenters of the acoustic emission are the positions where fracturing occurs. Then we integrated the acoustic emission data into a physically representative network model of the sample, which has a unit volume. The network model is a theoretical pore scale model with a 2D lattice geometry, where the pore space is characterized by a network of capillary tubes. We generate multiple such networks with different number of acoustic events integrated into it, so that we can capture all the different acoustic event density, the number of acoustic events per unit volume that occurs in the sample block during fracturing. We solve and upscale the pore scale network to predict the core scale permeability.

We hypothesize that if the acoustic event density at any location in the sample block is below a certain threshold value, we can predict the change in transport properties, such as absolute permeability compared to intact conditions using the principles of percolation theory. To test our hypothesis, we compare the predicted results with lab measurements. The permeability measurements (data) are obtained on core plugs that are extracted from the sample block after fracturing.

Our results indicate that in regions where the acoustic event density is below the threshold, there are only isolated fractures that are poorly connected, therefore there is no change in absolute permeability compared to intact conditions. But in sample region where this acoustic density is above the threshold value, there are enough fractures present for a percolation spanning cluster to occur. Hence, this region of the sample contains a macroscopic fracture that results in high permeability compared to the intact conditions.
References:


Click here to agree

Parallel 9-F / 375

Pore scale study of drying in porous media

Rui Wu

1 Shanghai Jiao Tong University

Corresponding Author(s): ruiwu@sjtu.edu.cn

Drying in porous media is of interest to many research and engineering fields, such as recovery of volatile hydrocarbons from underground oil reservoirs, remediation of contaminant soils by vapor extraction, and water management in gas diffusion layers (GDLs) of proton exchange membrane fuel cells (PEMFCs).

The drying process in a porous material is dependent on the structure and wettability of this porous material. In a porous material, the void spaces are composed of pores of various sizes. At the interface between a small and a larger pore, there exists a sudden geometrical expansion. Such sudden geometrical expansion increases the resistance to the menisci movement, and therefore is called the capillary valve effect. Because of this capillary valve effect, two types of pore invasion are revealed, i.e. bursting and merging invasion. We found that if the capillary valve effect is considered in the pore network model for drying of porous media, the modelling results will have a better agreement with the experimental data obtained from drying of a micromodel pore network.

For slow drying of a hydrophobic porous material where liquid flow is controlled by capillary forces and no liquid films exists, drying induced gas invasion in the porous material is a random process if bursting invasion dominates but shows a stable process when merging invasion dominates. For slow drying of a hydrophilic porous material, liquid films can form in the corners of pores. We will show there are two types of corner films. One is the continuous corner film, and the other is the discontinuous corner film. How the continuous and discontinuous corner films influence the drying process will be investigated in detail.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-D / 219

Pore scale velocity measurements in 3D – measurements in empty flow channel

Simon Franchini; Martin Blunt; Sam Krevor

1 Imperial College London
Corresponding Author(s): s.franchini15@imperial.ac.uk

In this project we aim to measure flow velocities in porous media. We demonstrate our method in a rectangular flow channel, for which a semi-analytical solution of the flow field exists. The flow channel is made of borosilicate glass and its refractive index is matched with the fluid. Upon doping of the fluid with microspheres, those particles can be tracked to reveal the velocity field of the fluid. Our work is based on the general defocusing particle tracking method (Barnkob, et al., 2015). This method allows the tracking of microspheres in fluids in three dimensions based on 2D microscope images. We extended the method to account for overlaying particle images and for aberration in the microscope optics. Previously, the method has been applied to investigate flow within one relatively thin measurement slice of 1510 x 1270 x 160 μm3 (Barnkob, et al., 2015). We show that multiple measurement slices can be stacked together, to cover a measurement volume of 2550 x 1440 x 2000 μm3. The resolution at which particles can be tracked in this volume is below 1 μm in the x- and y dimension. The out-of-focus locations of particles can be reconstructed with an RMSE of ~3 μm.

This method can directly be applied for measurements in porous media if the refractive index of the fluid and the solid are matched. It allows for high-speed, high-resolution measurements of flow velocities. The temporal resolution of the method is solely limited by the frame rate of the camera. In our case this is 1000 fps at full resolution.

References

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 377

Pore structure alteration of sands by microbially induced carbonate precipitation via denitrification

Author(s): Akiko Nakano\textsuperscript{Note}

Co-author(s): Tomoya Kakita

Corresponding Author(s): nakiko@agr.kyushu-u.ac.jp

Denitrification is one of the key microbial reactions for sandy soils to induce desaturation and calcium carbonate precipitation. As the replacement of urea hydrolysation for microbially induced carbonate precipitation (MICP), the effect by denitrification has been evaluated. Calcium carbonate precipitation and biomass production occur in soil through the reaction process and some of these accumulate in the pore space or on the surface of the soil particles. Due to the accumulation, reducing the porosity, permeability of the soil possibly reduces. Well understanding of pore structure alteration through the reaction makes possible to control permeability efficiently. This study evaluated pore diameter distributions of three sand samples before and after MICP treatment via denitrification by air intrusion method. By measuring air flow rate applying controlled air pressure into water saturated specimens of the sands, air permeability and pore diameter were calculated. Comparing non-treatment sands, the higher air pressure was required to push pore water against capillary pressure out of pore throats of sands after the treatment. The pore diameter distribution curves were slightly shifted to the smaller pore size range after the treatment. These results indicate that pore water retention ability of the samples was altered by the treatment.

References:
Acceptance of Terms and Conditions:
Click here to agree
Pore-Scale Modeling of Oil-Water Two-phase Flow in Tight Sandstones

Sen Wang¹ ; Qihong Feng¹ ; Farzam Javadpour² ; Ming Zha¹ ; Wei Zhang¹

¹ China University of Petroleum (East China)
² The University of Texas at Austin

Corresponding Author(s): wangsenai@126.com

With the advancement of multistage hydraulic fracturing technology, hydrocarbon production from tight reservoirs has exploded recently. Owing to its widespread nanopore, the permeability of tight sandstones are typically ~4 orders of magnitude smaller than conventional formations, thus leading to the breakdown of Darcy’s law within the complex nanoporous matrix. However, most of the existing research only concentrates on the single-phase flow in tight sandstones, whereas the transport of oil and water remains essentially not understood. Taking into account the tremendous effect of two-phase flow behavior on the accurate modeling of fracturing fluid flowback and production performance prediction, we studied oil-water two-phase flow in tight sandstones using pore network model.

Recent experimental studies suggested that because of the greater fluid-solid interactions, there exists a boundary layer (also termed immobile layer) near the pore walls, which decreases the pore radius and restricts fluid flow. We first developed a mathematical model, on the basis of previous experimental data, to describe the variation of boundary layer thickness in a circular micro/nano-tube. In comparison to previous models, which only accounted for the effect of pressure gradient, our model included more influencing factors, e.g., pore size, fluid types, temperature-dependent viscosity, etc., and showed excellent fit to the experiment measurements. Then we incorporated this formulation into a pore network model constructed for tight sandstone to simulate the single-phase water flow. The nonlinear correlation between flow rate and pressure gradient agreed well with the physical experiments on tight rock samples, which confirmed the validation of our model. As the pressure gradient increases, the apparent permeability of tight sandstone increases asymptotically and tends to approach a constant value corresponding to that without boundary layer effect.

We further proposed a pseudo-static pore network model to account for the effect of boundary layer on oil-water two-phase flow in tight sandstones. Because the thickness of boundary layer and estimation of hydraulic conductance are dependent on the pressure gradient, the nonlinear continuum equation was solved using an iteration algorithm to obtain the pressure distribution. We simulated the imbibition of water into the matrix of tight reservoirs. Our simulation results show that two-phase flow regions in the relative permeability curves of tight sandstones are always very narrow; that is, a tight rock sample has higher bound water saturation and residual oil saturation, which makes it more difficult to be exploited. We probe the effects of other properties, e.g., pressure gradient, pore/throat size distribution, coordination number, fluid viscosity, etc., on the two-phase flow behavior in tight sandstones. We suggested that the impact of boundary layer on fluid transport in tight sandstones should not be ignored. Our pore network model, which takes into account the effect of boundary layer on both single-phase and two-phase flows, have implications for tight oil but more generally for mass transfer through nanoporous media.

References:

Acceptance of Terms and Conditions:
Click here to agree

Pore-scale Experimental Investigation of Displacement Mechanisms during Flow of Non-Newtonian Fluids in Natural Porous Media

Abdelhalim Mohamed¹ ; Mahdi Khishvand¹ ; Mohammad Piri²
A large number of applications in science and engineering involve the flow of non-Newtonian fluids in naturally-occurring and synthetic porous media. Examples include flow processes that are related to enhanced oil recovery, underground waste disposal, and groundwater contamination. In the recent years, a growing number of studies have been dedicated to investigate a wide variety of viscoelastic fluids for use in enhanced oil recovery (EOR) from underground reservoirs. Pioneering field trials have indicated that the injection of viscoelastic fluids into a reservoir may provide sufficient increase in the capillary number to improve non-wetting phase mobilization and sweep efficiency compared to those of the traditional waterflooding. However, the pore-scale displacement mechanisms responsible for this improvement and the transport of fluids in porous media during viscoelastic fluid injection are poorly understood partly due its complex rheology. To the best of our knowledge, the current body of the literature has not distilled a clear image of the underlying displacement physics and essential physical relationships such as capillary desaturation curve during viscoelastic fluid injection. Hence, in this study, we address the trapping and mobilization of non-wetting phase during the flow of immiscible viscoelastic fluids.

We perform several sets of two-phase flow experiments on miniature water-wet Berea sandstone core samples at the microscale and using various Newtonian and viscoelastic aqueous phases. The experiments are performed on vertically oriented core samples at 4.12 MPa pore pressure and 5.52 MPa overburden pressure. The core initially saturated with water was subjected to a primary oil drainage (to establish Swi) followed by a waterflood during which the brine flow rate is increased stepwise. The core sample is scanned after each flood when no changes are observed in fluid configurations.

We use a two-phase miniature core-flooding apparatus integrated with a micro-CT scanner to directly visualize the complex morphologies of non-wetting fluid ganglia within natural porous media. This information is then used to study the effect of flow rate on oil mobilization over a wide range of flow rates corresponding to different regimes of the bulk viscoelastic flow behavior (i.e. shear flow and elongation dominated flow). Furthermore, pore-scale fluid occupancy maps during different flooding scenarios along with pore space characteristics, local fluid saturations, oil cluster size distributions, and in-situ wettability obtained from the tomography images are used to explain the observed capillary desaturation trends and shed light on the dominant displacement mechanisms under two-phase flow conditions.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-D / 330

Pore-scale Investigation of Solvent Based Bitumen Recovery

ZhenBang Qi¹; Lining Xu¹; Atena Sharbatian²; Ali Abedini¹; Adriana Guerrero³; David Sinton⁴

¹ University of Toronto Sinton Lab
² university of Toronto Sinton Lab
Current thermal methods for bitumen recovery are effective but require both environmental and economic performance improvements. Solvent based recovery method is an alternative to steam injection that has the potential to reduce greenhouse gas emissions associated with recovery. However, the pore-scale behavior of the solvent-bitumen system is very complex and poorly characterized to date. In the first part of the work, a high-pressure high-temperature micromodel with reservoir-relevant geometry combined with imaging tools is used to provide pore-scale of condensing solvent injection using propane and butane. The combination of two-phase dynamics and solvency at the condensing edge leads to significant bitumen production, similar in both propane and butane injections. In the liquid zone ahead of the condensing edge, butane results in dense, small, and immobile solvent-in-residue emulsions. In contrast, liquid propane produces larger emulsions with some mobility. Spectroscopy combined with fluorescence imaging indicates that the residual immobile emulsions in the butane case are bitumen heavy fractions, and largely asphaltenes. Motivated by the large amount of asphaltenes precipitated by liquid propane and butane, we extend the study to other commonly used hydrocarbon solvents for steam co-injection process, namely pentane, heptane, condensate, and naphtha. A set of microfluidic chips is uniquely designed to investigate the pore damage due to asphaltene deposition from different solvents in different pore geometries. It is observed that the pure pentane has the most damage to the reservoir while the naphtha produces the least amount of asphaltenes. Lastly, we evaluated the solvent-steam co-injection method inside the micromodel. Naphtha yields the best performance which can be attributed to both high azeotropic temperature and minimal asphaltene precipitation.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 60

Pore-scale Simulation Coupling Boundary Layer Effect And Media Deformation In Tight Formation

Mingqiang Chen1, Linsong Cheng1, Renyi Cao1, Chaohui Lv1

1 China University of Petroleum(Beijing)

Corresponding Author(s): 549135449@qq.com

Due to intense complexity and heterogeneity of pore and throat structure in tight formation, it’s very difficult for representation. In addition, as there abounds in large numbers of micro-nano pores and throats, boundary layer and media deformation effect on pore scale flow cannot be ignored. Therefore, an accurately representative pore network flow model which couples boundary layer and media deformation effect is in great need. An irregular 3D random network model which can characterize porethroat size distribution and connection in tight formation is proposed. Based on the representative pore network model, a flow mathematical model which couples both boundary layer and media deformation effect at the same time is developed. In order to verify the simulation result, micro-tube experiment is carried out. After validation, factors influencing pore scale flow in tight formation are studied, such as boundary layer effect, media deformation effect and pore network model structure parameters. Results show that: it is boundary layer effect rather than media deformation that leads to non-linear flow in tight formation. And the more intense the boundary layer effect is, the more apparent the non-linear flow phenomenon will be. In contrast, media deformation effect just results in smaller velocity at the same displacement pressure gradient and the linear relationship between the velocity and displacement pressure gradient is unchanged. In addition, as for the existence of boundary layer effect, absolute permeability in tight formation is no longer a constant, it varies with the displacement pressure gradient, which is different from conventional reservoirs. Meanwhile, media deformation just brings out the overall decline of absolute permeability which does not change the trend of the permeability versus displacement pressure gradient. As
coordination number in pore network model increases, connective paths grow larger, which eventually leads to the increase of absolute permeability. With the increase of aspect ratio, effective flow space is compressed, resulting in the decline of absolute permeability.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 606

Pore-scale Simulation of Residual Trapping of Supercritical CO2 via Cyclic Injections

Author(s): Yu Chen
Co-author(s): Albert Valocchi 2; Qijun Kang 3; Hari Viswanathan 3

1 University of Illinois at Urbana-Champaign
2 Univ Illinois
3 Los Alamos National Laboratory

Corresponding Author(s): ychenpku@illinois.edu

A recent experimental study [Herring et al., 2016] shows the potential of enhancing residual trapping of supercritical CO2 (scCO2) via cyclic injections. Two competing mechanisms were identified that impact residual scCO2 trapping: (1) the wettability of solid surfaces is altered due to direct contact with scCO2; (2) different capillary pressure results in different initial states of scCO2 fluid connectivity and topology prior to imbibition. To trap more scCO2 after imbibition, the former mechanism requires higher extent of scCO2 drainage while the latter requires lower extent of scCO2 drainage. Due to experimental limitations, control of local alteration of wettability in real rock is not possible; extensive and strict parametric study of cyclic injections are very expensive and difficult to achieve. Direct numerical simulation can largely overcome the above issues and reveal the relative importance of the two mechanisms. In this work, we employ our in-house developed lattice Boltzmann code to perform pore-scale simulations on micro-CT scans of Bentheimer sandstone to study the scCO2 trapping mechanisms in cyclic injections. Following the experimental procedure, we apply different capillary pressure to achieve different scCO2 configurations after drainage. Wettability is altered in the simulations on solid surfaces that are directly exposed to scCO2. The computation cost of parametric study is very high due to the multiple cycle injections and different combinations of parameters, thus manycore supercomputers are employed to perform the simulations.

Acknowledgements
This work was primarily supported as part of the Center for Geologic Storage of CO2, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science. Q.K. and H.V. acknowledge the support provided by LANL’s LDRD Program and the Department of Energy (DOE) Basic Energy Sciences program (DE-AC52-06NA25396). The supercomputers used in this work including TACC Stampede 2 and PSC Bridges both provided by XSEDE.

References:
Click here to agree

Parallel 4-H / 289
Pore-scale modeling of hydraulic fracture

Zhiqiang Chen¹; Moran Wang¹

¹ Tsinghua University Department of Engineering Mechanics

Corresponding Author(s): 145287789@qq.com

Hydraulic fracturing is one of primary engineering techniques to improve well productivity especially for unconventional reservoirs. Generally, there are two kinds of numerical models for hydraulic fracture simulation, continuum-based models and discontinuum-based models. In continuum-based models governing equations based on continuum theory are solved with single planar fracture assumption. However, in unconventional reservoirs this assumption breaks down, which results in the predictions by continuum-based models are not consistent with experiments [Al-Busaidi et al., 2005]. Firstly, complex rather than single hydraulic fracture is often observed in laboratory or field experiments [Wang et al., 2014]. Secondly, continuum-based models generally assume that hydraulic fracture is caused by tensile force at fracture tip, but shear-type seismic events are often recorded in experiments and even in some cases shear failure dominates the fracture behavior [Falls et al., 1992; Ishida et al., 2004].

In this work we develop a more accurate pore-scale hydro-mechanical coupled model, where the solid deformation and fracture behavior are simulated by discrete element method (DEM) and the fluid flow is solved directly by lattice Boltzmann method (LBM) at pore scale. To validate current hydro-mechanical coupled model, sphere sedimentation in Newtonian fluid is simulated, and the results agree well with that reported in literature. Then hydro-fracturing is simulated, attempting to answer the inconsistency between continuum-based model predictions and experiment observation. Simulation results show that strength heterogeneity of rock has a significant influence on hydraulic fracture geometry and the involved failure mechanism. In unconventional reservoir, rock strength heterogeneity is high, which leads to the complex fracture geometry and abundant shear failure events, but it is often ignored in continuum-based models. The origin of this strength heterogeneity arises from ubiquitous natural fractures in unconventional reservoir, which are sealed with different minerals. Thus, hydraulic fracture interaction with cemented natural fracture is simulated, which shows that strength contrast between cemented natural fracture and host rock plays an important role in hydraulic fracture propagation.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 1-G / 807

Pore-scale modelling of multiphase flow in porous media: considering wettability and disordered microstructure

Yixiang Gan¹

¹ The University of Sydney

Corresponding Author(s): yixiang.gan@sydney.edu.au
Multiphase flows in disordered porous media have a significant influence on many industrial applications, such as unsaturated soil mechanics, carbon geo-sequestration, and oil recovery. In this paper, we discuss two aspects of the problem, namely, (1) wettability at dynamic conditions and (2) disordered microstructures.

First, to simulate surface tension, wetting effects as well as dynamic contact angle at the pore-scale, a smoothed particle hydrodynamics (SPH) model with inter-particle force and modified solid-liquid interface formulation is applied. A newly introduced viscous force at solid-liquid interface is implemented to generate the rate dependent behaviour of contact angle with moving contact line, which can reflect the realistic interaction between different phases based on physical quantities. The dynamic contact angles are simulated under various moving contact line speeds and the correlation between corresponding capillary numbers are further analysed. The results are in good agreement with experimental observations under dynamic loading conditions and the effectiveness of the modified model is demonstrated.

Moreover, to study the effects of disordered pore networks on drainage characteristics, we used both numerical simulations (OpenFOAM) and physical experiments. The simulations covered a wide range of non-dimensional number, considering wettability, viscosity and surface tension. An improved Bond number equation for disordered porous media was proposed to capture the residual saturation as a function of gravity for different pore structures. Furthermore, we redefined the calculation procedure of the disorder parameter Iv, based on Voronoi tessellation, which is found to have a negative and linear correlation with the residual saturation for given gravity-driven drainage conditions. A qualitative agreement has been found between the simulation and experimental observations.

These preliminary results demonstrated the potential of using these proposed methods for accounting the pore-scale effects, including the hysteretic contact angle and disordered pore structures, and for simulating multiphase flows in porous media under various loading conditions.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-F / 847

Pore-scale simulation of kinetic calcite pore cement dissolution in a µCT sandstone sample

Christian Hinz1 ; Frieder Enzmann1 ; Michael Kersten1

1 University of Mainz, Institute for Geosciences

Corresponding Author(s): christian.hinz@uni-mainz.de

We present a reactive fluid dynamics modelling approach coupling flow physics and geochemical calculations at pore scale resolution. A model workflow combining numerical solvers has been developed according to the operator splitting approach and the Lagrangian transport method. The FlowDict module of the GeoDict software package (Math2Market GmbH, Germany) iteratively computes the flow field of a given three dimensional porous geometry by applying the Navier Stokes-Brinkman LIR solver (Linden et al., 2015). The AddiDict module simulates the advective and diffusive motion of virtual particles. These particles carry aqueous solutions, which mix with pore fluid solutions and react once bouncing at surfaces resulting in dissolution and/or precipitation of mineral phases at the sub-voxel scale. Kinetically controlled geochemical equilibrium calculations are performed by the C++ library of the open-source code PHREEQC (USGS). In addition, it is planned to implement Reaktoro (Leal et al., 2017) in order to further increase the possibilities and performance of the existing geochemical workflow. Our code embeds the prior mentioned modules into a time loop for sequentially simulating pore-scale reactive transport at changing solid matrix volume. GeoDict control and data files are automatically accessed to communicate the processed geochemical data. Multiple MPI-processes and OpenMP threads are applied to provide an efficient performance of the C++ reactive transport code.
In a μCT sandstone structure, kinetic dissolution of calcite pore cements is simulated. Therefore, an inflowing acidic solution continuously replaces the equilibrium pore fluid triggering dissolution reactions at calcite surfaces. Results show effects of local pore space alterations on the continuously changing hydromechanical transport parameters calculated according to the Digital Rock Physics concept.

References:
Click here to agree

Poster 4 / 769
Pore-scale simulation of mass transfer across scCO2-water interface using phase-field method
Farzad Basirat¹ ; Zhibing Yang² ; Auli Niemi³

¹ Department of Earth Sciences, Uppsala University
² Wuhan University
³ Uppsala University
Corresponding Author(s): farzad.basirat@geo.uu.se

Interfacial mass transfer between scCO2water in porous media is a key process for dissolution and mineral trapping of CO2 during geological storage of CO2. Recently, both core- and pore-scale drainage and imbibition experimental studies have shown non-equilibrium dissolution of scCO2 and an extended depletion of residual scCO2 (Chang et. Al. 2016, 2017). For better understanding and quantifying the dissolution process of we need models to capture the rate-limited dissolution of scCO2 at the pore level. In this work, we develop a simulation model to capture two-phase flow and interfacial mass transfer at the pore-level. We used a continuum approach for interfacial mass transfer along with a phase-field method as an interface-capturing technique for the two-phase flow system. The model has been applied to a single pore for validation and subsequently to numerical simulation of 2D homogeneous micromodel experiments. The preliminary results show that the model can capture the mass transfer between the two phases and at the same time the interface adjustment.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-C / 687
Poroelastic properties on metal foams submitted to high pressure
Enrique Peña De la Paz¹ ; Elsa de la Calleja² ; Ignacio Figueroa²

¹ Instituto de Investigaciones en Materiales
² Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México
Corresponding Author(s): enriquepdp.fi@gmail.com

The metallic foams are a novel possibility to impact significantly the design of materials taking into account the wide technological applications [1,2]. In this work the procedure to manufacture metallic foams with controlled porosity is presented. A high pressure cell is used to submit the metallic foams to reservoir conditions, which imply high pressures and high temperatures. The injection of the optimal fluid in metallic foams increase the pore pressure which induces a dilation of the foam [3]. These effects are described with poroelastic deformation quantities. The porous deformation is directly measured by image analysis and the well-known mechanical properties are calculated based in basic theoretical models. The aim of the present work is describe the poroelastic behavior of metallic foams [4] when they are submitted in reservoir conditions. The permeability and porosity are measured experimentally and the Carman-Kozeny [5] model is used to model our results. Our experimental results indicate that metallic foams poses high structural stability even if they are mechanically perturbed.

References:
5 Dante Hernandez-Diaz, Oscar Chavez, Alberto Beltran, Armando Garcia, Baltasar Mena, and R. Zenit, Experimental study of the effect of wettability on the relative permeability for air-water flow through porous media (Submitted 2017) Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 933

Poroelastic response of a stationary fracture subjected to a constant fluid flux

Author(s): Zhiqiang Fan

Co-author(s): Rishi Parashar

\(^1\) Desert Research Institute

Corresponding Author(s): zhiqiang.fan@dri.edu

Fracture permeability that governs fluid flow within fractures is highly sensitive to fracture aperture that is affected by the fluid pressure on the fracture surface and far filed in situ stress. Previous research focused on fracture behavior in poroelastic medium with only stress and pore pressure boundary conditions on fracture surface. A more general solution should take into consideration a fluid flux boundary which is more suitable for fluid injection/withdrawal. We present a poroelastic model coupling geomechanics with fluid flow to investigate the transient fracture aperture of a single fracture subjected to a constant fluid flux in a poroelastic rock matrix. Load decomposition technique is used to separate the contributions to the aperture changes and stress intensity factor at the crack tip from the mechanical loading and fluid flux. Laplace transform is employed to derive a pair of singular integral equations for the coupled crack opening displacement and pore pressure. A semi-analytical solution is obtained in the Laplace domain and numerical results in the time domain is obtained via the Stehfest inversion approach. Asymptotic expressions for short term undrained and long term drained fracture aperture and stress intensity factor are derived. Based on linear fracture mechanics, the critical fluid flux required to propagate the fracture is determined. From the results we can see that the mechanical loading keeps the fracture open but the pore pressure loading induced by the fluid flux tends to close the fracture. The transient fracture opening is determined by the net loading imposed on the fracture surface. We also note that the stress intensity factor
differs significantly from that when the fracture is subjected to a constant pore pressure. The present solution may provide useful guidance for hydraulic fracturing design and serve as a new benchmark solution to validate numerical code development in fully coupled poroelasticity.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-F / 142

Porosity and permeability change of Lower Tuscaloosa and Marine Shale formations (Mississippi, USA) induced by CO2 injection: a numerical study

Author(s): Liwei Zhang

Co-author(s): Yee Soong ; Robert Dilmore ; Yan Wang ; Xiaochun Li

1 Institute of Rock and Soil Mechanics, Chinese Academy of Sciences
2 National Energy Technology Laboratory

Corresponding Author(s): zlw_85@foxmail.com

A reservoir-scale numerical model was developed with the use of multi-phase reactive transport code TOUGHREACT to estimate porosity, permeability and mineral composition changes of Lower Tuscaloosa (LT) sandstone formation and Marine Shale (MS) caprock overlying LT formation when CO2 is injected into LT formation. The reservoir-scale numerical model was developed based on geological settings of LT and MS formations at Plant Daniel CO2 storage test site, Mississippi, USA. Another core-scale reactive transport model was developed with the use of reactive transport code CrunchFlow to predict permeability evolution of small LT and MS samples when exposed to CO2-saturated brine in the laboratory, and the permeability and solution chemistry results from the model were compared with experimental data to validate important modeling parameters (equilibrium constants (Keq), reaction rate constants (k) and n in the Verma-Pruess permeability-porosity relation) that were used in the reservoir-scale simulation. Both the reservoir-scale model and the core-scale model predict precipitation of amorphous silica (SiO2, am) and kaolinite in the pore space of LT rock when interacting with CO2-saturated brine. Dissolution of chlorite and feldspar is also predicted. However, mineral precipitation and dissolution are limited in both LT and MS formations after interacting with CO2-saturated brine for 130 years, and porosity and permeability changes of LT and MS formations caused by mineral precipitation/dissolution are minimal.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-E / 822

Porosity effects on phase diagram of gas condensate mixture

Vasily Pisarev ; Stepan Zakharov

1 Joint Institute for High Temperatures of RAS

Corresponding Author(s): pisarevvv@gmail.com
A phase diagram of methane+n-butane mixture is investigated by the means of molecular dynamics (MD) simulations. The system exhibits retrograde condensation behavior above 191 K in some range of methane molar fractions. A vapor-liquid equilibrium curve for mixtures is calculated with TraPPE-UA united-atom forcefield 1, TraPPE-EH [2] and OPLS-AA [3,4] all-atom forcefields. The forcefields show good agreement with experimental vaporization curves of pure hydrocarbons. They also reproduce well the composition of liquid phase in binary mixtures as a function of pressure at isotherms, while some discrepancies from experimental data are observed in the saturated vapor compositions. The TraPPE forcefields show better agreement with experimental vapor-liquid equilibrium data than OPLS. The TraPPE-EH accuracy is comparable to that of cubic equations of state. The effects of nanoscale porosity on mixture phase diagram are qualitatively studied. The saturation curves in slit pores with Lennard-Jones walls are calculated. We considered two sets of wall-molecule interaction parameters and two pore widths. It is shown that nanopores may shift the coexistence curve. At certain wall-molecule interaction parameters, a significant widening of the pressure range of the retrograde condensation is found. This effect may hinder gas extraction from the rocks with a large fraction of nanopores. The work is supported by the Russian Science Foundation (grant no. 17-79-20391).

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 827

Porous Structure Reconstruction Using Convolutional Neural Networks

Yuzhu Wang1\textsuperscript{a} ; Wang Yudong\textsuperscript{1} ; Sheik Rahman\textsuperscript{2}

\textsuperscript{1} UNSW

Corresponding Author(s): wangyuzhu2103418@163.com

A three-dimensional (3D) high resolution inner structure of rock sample is premise for pore-scale flow simulation of reservoir. $\mu$-CT is considered to be the most direct way to obtain the 3D inner structure of porous media without deconstruction. However, its micrometer resolution limits its application in characterization of small structures such as nano-pores and channels which are critical for fluid transportation. An effective strategy to solve this problem is applying numerical reconstruction methods to improve the resolution of porous structure extracted from $\mu$-CT image. In this paper, we introduce a convolutional-neural-networks reconstruction (CNNR) method to reconstruct high resolution porous structure based on low resolution tomographic $\mu$-CT image and high resolution SEM image(s). The proposed method is carried out through four steps. Firstly, a rock sample is scanned by $\mu$-CT to build a relative low resolution 3D tomographic image. Then one or more sections in the rock sample are selected to be scanned by SEM to obtain the high resolution 2D images. After that, the high resolution segmented SEM images and their corresponding low resolution $\mu$-CT slices are used to train the CNN model. Finally, the trained CNN model is used to reconstruct the whole low resolution 3D $\mu$-CT image. Due to the SEM images are segmented and have higher resolution than that of $\mu$-CT image, this algorithm integrates the super resolution and segmentation process together. The input data is low resolution tomographic $\mu$-CT image and the output is high resolution segmented porous structure. The experimental result shows that the proposed method is able to achieve the state-of-the-art performance.

References:
Porous media deformation and self-structuring under capillary bulldozing

Guillaume Dumazer¹ ; Bjørnar Sandnes ² ; Monem Ayaz³ ; Knut Jørgen Måløy¹ ; Eirik Flekkøy¹

¹ University of Oslo, Porous Media Laboratory
² College of Engineering, University of Swansea
³ Institut de Physique du Globe de Strasbourg

Corresponding Author(s): guillaume.dumazer@fys.uio.no

An experimental observation of the structuring of a granular suspension under the progress of a gas/liquid meniscus in a narrow tube is reported here. The granular material is moved and compacts as a growing accumulation front. The frictional interaction with the confining walls increases until the pore capillary entry pressure is reached. The gas then penetrates the clogged granular packing and a further accumulation front is formed at the far side of the plug. This cyclic process continues until the gas/liquid interface reaches the tube’s outlet, leaving a trail of plugs in the tube. Such 1D pattern formation belongs to a larger family of patterning dynamics observed in 2D Hele-Shaw geometry. The cylindrical geometry considered here provides an ideal case for a theoretical modelling for forced granular matter oscillating between a long frictional phase and a sudden viscous fluidization.

References:

Parallel 11-E / 80

Porous media evolving mechanism, theory and its applications in Hot Dry Rock geothermal energy and oil shale

Yangsheng Zhao¹

¹ Taiyuan University of Technology

Corresponding Author(s): y-s-zhao@263.net

A wide range of solid media gradually evolve into porous media containing a large number of pores, and sometimes voids and fractures, after a single or several coupled physical and chemical actions. This is a very common phenomenon in nature.

It is extremely important in the field of science, engineering and biomedicine on the rise of the research direction and research subject.

The evolution mechanism of porous media is very complex, we consider roughly divided into three categories: ① Natural evolution, ② Artificial evolution, ③ Natural–artificial evolution.

The experimental results: 1) Process of dissolving of salt, evolving properties of solid skeleton; 2) Process of heating, the crack feature of granite (HDR reservoir); 3) Process of pyrolysis, pore and crack feature of oil shale.

Theory: to study the pore and fracture occurrence, development process, the description of the pore morphology and its connected, and control equation for seepage mass transfer, heat transfer in porous media, describing the process of evolution. We put a few mathematical model, i.e. 1) The
coupled math. model of solid deformation and gas seepage in methane in coal bed mining; 2) The coupled math. Model of solid deformation, heat transport and seepage in HDR exploitation; 3) the coupled mathematical model of solid deformation, heat and mass transport and seepage in oil shale exploitation. 4) pore and fracture double media percolation theory of evolving from impermeability to permeability

Application in China: 1) Geothermal of Hot Dry Rock exploitation, introduction of HDR geothermal resources in China, such as geothermal development, nuclear waste disposal, mechanism and development of oil and gas, groundwater, earthquake prediction. Engineering exploration and development case such as Gongshe County in Qinghai Prov and yangbajing in Tibet Prov.

2) Oil shale exploitation by injection water vapor in in-situ. pilot test study in large sample, Decorate 20 drilling, 150m of ground pressure, a few of hole the continuous injection of water vapor, another holes discharge by pyrolysis of oil and gas and water vapor steam exhaust. In the process of test, measured pressure, temperature, deformation, f acoustic emission events, products change of properties and quantities.

introduce to Xinjiang prov. oil shale geological occurrence conditions and develop technology plan.

References:

Acceptance of Terms and Conditions:

Click here to agree

---

**Poster 4 / 1105**

**Porous media for thermochemical energy storage: experimental investigation on structural changes of reactive materials**

**Author(s):** Jana Stengler¹

**Co-author(s):** Marie Gollsch ¹; Julius Weiss ¹; Marc Linder ¹

¹ German Aerospace Center (DLR)

**Corresponding Author(s):** jana.stengler@dlr.de

The use of gas-solid reactions for thermochemical energy storage has been widely discussed in literature. Still, the question of handling a reacting solid on a technically relevant scale is not solved yet: structural changes within the porous solid media need to be considered when designing high-power storage reactors for commercial applications.

In an experimental study, we have successfully demonstrated the applicability of strontium bromide and water vapor as a reacting couple: 

$$\text{SrBr}_2\cdot\text{H}_2\text{O} (s) + \Delta H \rightleftharpoons \text{SrBr}_2 (s) + \text{H}_2\text{O} (g)$$

A sample mass of around 100 g of hydrated salt was investigated with regard to its use as thermochemical energy storage material in the temperature range of 200 °C to 250 °C. In our experimental work, we found that the macroscopic and the microscopic properties of the solid bulk material change considerably during the first reaction cycles: the primary particles agglomerated, and the overall volume of the porous bulk significantly increased within 27 dehydration/re-hydration cycles. Structural changes in the porous media influence the progression of the gas-solid reaction: A change in bulk material permeability directly affects the vapor mass transfer. Furthermore, the observed structural changes can lead to a reduced bulk thermal conductivity and thus have a negative effect on the thermal performance of a storage reactor.

The aim of our work is to enhance the understanding of the decisive factors for the thermal power of a thermochemical reactor and to quantify their impact in wide pressure and temperature ranges (1 kPa – 0.6 MPa, 100 – 320 °C). Our main objective is the consideration of aging effects of the reactive bulk material when deriving layout rules for the design of high-performance reactors.

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 8-B / 1005

Porous medium theory in patient pre-treatment planning

Author(s): Hooman Farsani

Co-author(s): Marcus Herrmann; David Frakes

1 Arizona State University

Corresponding Author(s): farsani@asu.edu

Physicians often face multiple possible strategies treating a specific disease and it is crucial to have a predictable numerical methodology that can help with selection of the best option. Brain aneurysms are a result of a weakened blood vessel wall that, if not treated well, can have a lethal rupture. To prevent the rupture, multiple devices are available, including coils and flow diverters. These devices impede the flow of blood for better coagulation; thus, significantly reducing the chances of rupture. However, the choice is patient specific and a numerical investigation of these devices on hemodynamics is necessary. Computational fluid dynamics (CFD) is often used to assess the performance of these devices and their effect on hemodynamics. Unfortunately, due to the complexities associated with a conventional CFD study including the extremely time-consuming meshing procedure and high computational cost, this technique has not received the attention it deserves. To bypass the complexities mentioned above, researchers have suggested the use of a porous medium approach [2]. In this approach, the explicit geometry of the device is replaced by a homogeneous porous region. This avoids the need for a body fitted mesh and therefore extremely simplifies the meshing procedure and reduces the CFD run time. However, the main challenge is the non-uniform geometry of these devices that invalidates the homogeneity assumption and needs a rather intricate approach. To address this challenge, we propose a novel way that considers the heterogeneity of the devices while not sacrificing the accuracy. The device is replaced by a non-uniform map of permeabilities and porosities and the Navier-Stokes equations are solved by incorporating Darcy’s law.

An area that yet must be addressed is the blood coagulation during treatments, as it leads to a dynamic change in porosity and permeability of the domain. Thus, the heterogeneous map has to be dynamically updated which requires a more comprehensive approach to consider for this complex phenomenon. Additionally, the force on the porous region imposed by the flow of blood can lead to deformations in the region which then can alter the hemodynamics. This approach and its challenges pertain to the study of air flow in the lungs. To understand the flow behavior in airways to improve the drug delivery, airways are often considered to be porous as it would be rather challenging to mesh the pathways via a conventional CFD mesher. However, as there are multiple length scales available in the lungs, more research needs to be done to introduce a multi-scale porous medium approach for this purpose. Moreover, the fact that the movement of walls can have significant effect on the flow of air or blood, a model which considers the movement of the porous region is necessary. In summary, we believe that the work presented in this study has addressed a significant challenge in the application of porous medium theory in biomedical related studies. Nonetheless, the aforementioned challenges open doors for research areas that lead to a more comprehensive modeling pipeline using the porous medium theory.


References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-H / 423
Precipitation and dissolution of cement minerals in sandstone: Opportunities and limitations of pore and plug scale flow analysis for reactive transport modelling approaches

Johannes Kulenkampff¹; Lotfollah Karimzadeh¹; Cornelius Fischer¹

¹ HZDR

Corresponding Author(s): c.fischer@hzdr.de

Reservoir properties of sandstones are controlled by precipitation and dissolution reactions at the pore walls. Both, the formation and dissolution of cement minerals are responsible for the complex pattern formation of porosity and permeability in reservoir rocks. At the scale of drilled core sections (plugs), experimental and analytical approaches utilize positron emission tomography (PET) with radiotracer (Kulenkampff et al. 2016). Resulting spatiotemporal concentration distributions provide quantitative insight into fluid flow and diffusion parameters. The sensitivity is in the picomolar range of the utilized radiotracers and the spatial resolution is about 1 mm. Thus, mechanistically-important surface features such as etch pits or growth hillocks and their evolution during reaction are not yet part of the direct analysis of the flow field. Here, we present an approach based on existing information about the complex crystal surface morphology and rate evolution (Fischer & Lutte 2017). We utilize artificial materials that are produced by 3D printing capabilities. Such an approach using PET analysis of sequences of machined surfaces in flow-through experiments provides quantitative insight into the local stability vs. temporal heterogeneity of fluid flow close to reacting surfaces. The measured flow velocity data from PET are implemented into reactive transport models and compared to calculations focusing on small-scale surface reactivity. We discuss the resulting size and complexity of surface rate patterns.

References:
J. Kulenkampff, M. Gründig, A. Zakhnin and J. Lippmann-Pipke (2016): Geoscientific process monitoring with positron emission tomography (GeoPET). Solid Earth, 7: 1217-1231

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 664

Predicting fracture permeability through pore-scale simulations

Qinjun Kang¹; Jeffret D. Hyman¹; Satish Karra¹; Luke P. Frash¹; Phong Nguyen²; J. William Carey¹; Hari Viswanathan¹

¹ Los Alamos National Laboratory
² Los Alamos National Lab

Corresponding Author(s): qkang@lanl.gov

A three-dimensional lattice Boltzmann model (LBM) is used to predict fracture permeability. The LBM is first verified by comparing the predicted permeability of a straight pipe with a rectangular cross section with the analytical solution. Excellent agreement is achieved for various aspect ratios of the cross section. Then the LBM is used to simulate single phase fluid flow in fractures whose geometries are obtained from the segmentation of triaxial direct-shear experiments conducted on shale. The experiments provide shear fracture geometry and permeability as a function of confining stress and fracture displacement. The pixelated representation of the fractures is directly used in the LBM simulation, while body-fit meshes are generated for solving the incompressible Navier-Stokes Equation using OpenFoam. Predicted permeabilities using both numerical methods are compared with each other and in relation to experimental observations. In addition, we compare computational efficiency of the numerical methods.
We simulate multiple fracture geometries under different stress conditions and the dependence of fracture permeability on contact area is investigated. The results are also used to investigate universal scaling relationships between fracture stiffness and fluid flow as proposed by Pyrak-Nolte and Nolte (Nat. Comm. 2016).

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-B / 133

Prediction of the thermal conductivity of porous building materials with nanoscale pore size distributions

Author(s): Wouter Van De Walle

Co-author(s): Hans Janssen

1 KU Leuven, Building Physics Section

Corresponding Author(s): wouter.vandewalle@bw.kuleuven.be

Porous materials find frequent use in numerous thermal applications, offering a strong reduction of the total heat flow. Typical applications can be found in the automotive industry and aerospace engineering for the protection of sensitive components, but also in the building industry where heat losses through the opaque building components still account for a large part of the needed heating energy. Therefore, recent research activities have focused on the development of several new types of porous materials, i.e. vacuum insulation and aerogels, showing strongly reduced thermal conductivities compared to conventional insulating materials. Their improved performance is mainly attributable to their microstructure, composed of pores and matrix walls with nanoscale characteristic dimensions, rendering the classic Fourier diffusion heat law no longer valid. Indeed, at decreasing length scales and pressures, the heat flow behavior is known to shift to the Knudsen diffusion regime, resulting in reduced conductive heat transfer through the gaseous and the matrix phase. A more thorough understanding of the impact of these microstructural parameters on the total heat flow through the material could hence lead to a significant optimization of insulating materials. However, current numerical studies are often based on simplified analytical models and microstructures or focus on only one form of heat transfer.

In this study, a recently implemented pore-scale model for studying heat transfer in conventional cellular porous materials is expanded for studying materials with nanoscale features or reduced gas pressures. The model is based on 3D voxel images of the microstructure, thus incorporating the true microstructural parameters. The nanoscale ballistic behavior of the energy carriers in the gaseous phase is modelled by defining local thermal conductivities based on the kinetic theory. The reduced local effective mean free path is calculated using several geometrical parameters, considering both the shape and the size of the pore structure. Hence the model allows for an efficient simulation of the heat flow through the material, while implementing the Knudsen diffusion locally at the pore scale. The model is verified using existing analytical models and simple microstructures, showing good agreement. Finally, the model is used to make a preliminary study on the relative impact of several microscale parameters, showing the potential improvement of these new materials compared to conventional materials.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 1108
**Pressure drop and non-intrusive velocity measurements in packed beds**

Thien Nguyen\(^1\); Ethan Kappes\(^1\); Stephen King\(^1\); Yassin Hassan\(^1\); Victor Ugaz\(^1\)

\(^1\) Texas A&M University

**Corresponding Author(s):** thien.duy.ng@tamu.edu

Flows in packed beds are encountered in many engineering applications, such as solar thermal energy storages, chemical catalytic reactors, petroleum and civil engineering, magnetic refrigerators, biological tissues, and pebble-bed nuclear reactors.

Critical challenge of designing packed beds involves understanding the total pressure loss, complex flow fields, heat and mass transfer phenomena occurring within the interstitial regions. Unfortunately, complex geometries and randomly connected void spaces within packed beds have hindered efforts to characterize the underlying transport phenomena.

Geometrical complexity inside of a randomly packed bed represents a challenge to experimental and computational efforts in order to construct transport models that have been previously built upon volume averages of micro-scale parameters, however, should accurately capture the flow behaviors.

Fully leveraging the advantages of this type of packed beds requires a fundamental understanding of flow topology within the randomly packed sphere beds. Multiple points or full-field measurements of flow characteristics at a high level of spatial and temporal resolutions are needed to fully map the complex flow patterns and to provide data at high spatial density to permit accurate volume averaging in the pebble bed.

Texas A&M University is conducting isothermal measurements of pressure drops, flow measurements in a randomly packed spheres experimental facility to support the research on advanced nuclear reactors sponsored by Department of Energy (DOE). The main purpose of these tests is to perform high spatial and temporal resolution measurements, and use the obtained results for code validation and model development.

In this poster, we present our experimental results from pressure drop and non-intrusive velocity measurements in different facilities of randomly packed spheres at various porosities and Reynolds numbers.

Pressure drops across the axial length of a versatile facility were measured by high accuracy pressure transducers at various modified Reynolds numbers, and friction factors were accordingly computed. The obtained experimental results were compared and in a good agreement with previous studies available in literature.

High-fidelity velocity measurements at the pore scales and near the wall boundary in a facility of packed spheres were performed by featuring a combined approach of matching-refractive-index (MRI) and laser-diagnostics, such as Time-resolved Particle Image Velocimetry (TR-PIV) and Time-resolved Stereoscopic PIV (TR-SPIV). This approach allows us to non-invasively probe the flow within packed spheres at the microscopic scales with high temporal and spatial resolutions. Statistical results including mean velocity, root-mean-square velocity and Reynolds stress, computed from the TR-PIV and TR-SPIV measurements are illustrated. Effects of wall enclosures and Reynolds numbers to the flow patterns are investigated. Finally, we applied Proper Orthogonal Decomposition analysis to extract coherent flow structures in the near-wall and far-wall regions of the packed beds.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

Parallel 2-F / 310
Probing foam’s texture in porous media with Neutron scattering and X-ray tomography

Author(s): Chakib OUALI

Co-author(s): Elisabeth ROSENBERG ; Loïc BARRÉ

IFP Energies Nouvelles

Corresponding Author(s): chakib.ouali@ifpen.fr

Foam injection is believed to be a promising technique to enhance oil recovery. One of the key characteristics of the foam and its rheology in porous media is its texture which describes the spatial distribution and size of the gas bubbles. Yet, the description of the texture of a foam confined in a real porous medium is a challenging issue because conventional methods do not have adequate spatial and temporal resolution or are not adapted to opaque media. The foam texture has been extensively investigated in 1D and 2D micromodel experiments or from bubble size measurements outside the core. Until now, in-situ measurements of foam’s texture during foam flow in porous media has not been experimentally investigated.

Small Angle Neutron Scattering (SANS) is a powerful technique to probe the microstructure of Bulk foams (from the nanometer scale to the micrometer scale). We propose here to extend this technique to characterize the foam in a real 3D granular media by using contrast matching conditions. In this study, SANS acquisitions are made in a specific cell allowing pressure drop measurements and control of flow rate injections. The foam made of Sodium Dodecyl Sulfate (SDS) and Nitrogen is generated in-situ by co-injection of gas and the surfactant solution. The porous media are made of fused silica grains, prepared and sieved according to specific targeted grain distributions. The geometrical characteristics of the pore network are extracted by image analysis from X-ray microtomography and compared to the calculated bubble size. Foam texture is measured as a function of foam quality, interstitial velocity and grain size distribution.

In parallel, we run experiments on a Bentheimer core using a CT X-ray scanner in which pressure drop measurements and saturations are measured for different foam qualities and interstitial velocities. We used a methodology to trace back to the in-situ texture. The two experimental approaches are compared in terms of foam generation, flow and in-situ texture.

References:

Click here to agree

Parallel 2-F / 100

Probing the Effect of Oil Type and Saturation on Foam Flow in Porous Media

Reza Amirmoshiri ; Yongchao Zeng ; Zeliang Chen ; Sebastien Vincent-Bonnieu ; Rouhi Farajzadeh ; Sibani L. Biswal ; George J. Hirasaki

Rice University
Shell Global Solutions International

Corresponding Author(s): moshiri@rice.edu
The foam efficiency in the oil displacement processes is governed by foam stability which is generally reduced with the presence of oil. In this study, we investigate the effect of oil type and saturation on foam strength in Berea sandstone cores using coreflooding and nuclear magnetic resonance (NMR) imaging. Foam quality scan in the presence of remaining hexadecane showed higher apparent viscosities compared to the oil-free case except at very high foam qualities. We analyzed the foam-induced oil displacements mechanisms from the saturation profiles, measured by NMR, and determined the relative significance between the increased capillary number and the micellar solubilization. Furthermore, we carried out foam-oil co-injection tests with hexadecane, octane, and reservoir crude oil to correlate foam apparent viscosity with the oil saturation. Under our experimental condition, it was determined that with the increase in oil saturation, foam apparent viscosity first decreases because of foam weakening with oil; and then increases due to oil emulsification with the surfactant solution. The observed trend was similar for octane and hexadecane. However, octane resulted in higher foam destabilization and lower emulsification.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-E / 713

Production Data Analysis from Unconventional Reservoirs with a Novel Data-Driven Drainage Volume Approach

Zhenzhen Wang\(^1\); Michael King\(^1\)

\(^1\) Texas A&M University

Corresponding Author(s): zhenzhenwang007@gmail.com

Understanding how pressure fronts propagate (diffuse) in unconventional reservoirs is fundamental to transient flow analysis as well as reservoir drainage volume estimation. We have developed an alternative approach to the solution of the 3-D diffusivity equation by directly solving the propagation equation for the “pressure front” of the transient solution. The pressure front equation is an Eikonal equation, which is obtained from the high frequency asymptotic limit of the diffusivity equation in heterogeneous reservoirs and whose properties are well developed in the literature. Most importantly, the Eikonal equation can be solved very efficiently by a class of solutions called the Fast Marching Methods for a “diffusive time of flight” that governs the propagation of the pressure front in the reservoir. The diffusive time of flight can be used as a spatial coordinate to reduce the 3-D diffusivity equation into an equivalent 1-D formulation, leading to a simplified method for rapid reservoir modeling.

Based on this theory, we may further introduce a novel data-driven approach for production analysis of unconventional reservoirs without the traditional rate transient and pressure transient (RTA/PTA) assumptions of specific flow regimes. Our approach uses a transient generalization of the Matthews-Brons-Hazebrook method for the FSS drainage volume which relies on a \(w(r)\) function to characterize the flow geometry from the transient drainage volume. Together with a calculated instantaneous recovery ratio, it has been successfully used to rank refracturing candidates and to obtain optimal fracture spacing. Given well pressure and flow rate data, we can calculate the transient well drainage volume with time. The time evolution of the drainage volume can be inverted to derive the \(w(r)\) function which then provides a high resolution diagnostic plot that can be used for quantitative analysis to obtain fracture surface area, matrix properties, stimulated reservoir volume (SRV), and additional reservoir and fracture characteristics that are not apparent in the usual rate and pressure transient analysis techniques.

We have applied our methodology to field examples from the Montney and Eagleford shales. The comparison to standard RTA/PTA shows linear flow and fracture interference features more clearly than conventional RTA/PTA. It also provides detailed characterization of complex non-planar hydraulic fracture geometry, partial completion effects, the development and growth of the SRV, leading to the estimation of future decline rate and ultimate recovery.
The major advantage of the proposed approach is the data-driven model-free analysis of production data without the presumption of specific flow regimes. It provides a simple and intuitive understanding of the transient drainage volume and instantaneous recovery efficiency, irrespective of the complexity of the geometry of the reservoir depletion.

References:


Parallel 11-E / 306

Production decline behaviors analysis of a vertical well with natural water influx/waterflood

Mingqiang Wei¹ ; Yonggang Duan² ; Qingxuan Chenª ; Morteza Dejam³

¹ Southwest Petroleum University
² Southwest Petroleum University
³ University of Wyoming

Corresponding Author(s): weiqiang425@163.com

In petroleum engineering, the production decline type curves for the analysis and interpretation of production data has been considered as a robust method to obtain the flow parameters, and original gas in place etc. However, most of the previous production decline analysis model focused on primary depletion with closed boundary, rather than secondary depletion with water influx/waterflood. Thus, in this paper a model considering the water influx/waterflood with ramp rate case at the external boundary is developed. Subsequently, based on the material balance equation in consideration of the water influx/waterflood effect, the functions of Blasingame decline type curves for a vertical well with water influx/waterflood is derived and obtained so as to extend the theory of Blasingame production decline analysis to influx/waterflood reservoir. Further, advanced Blasingame production decline type curves of a vertical well in water influx/waterflood reservoirs are plotted through Stehfest numerical inversion algorithm and computer programming. Four flow regimes, including early unsteady flow regime; primary depletion flow regime; second unsteady flow regime; system pseudo steady flow regime, are recognized. Compared with Blasingame type curves without water influx/waterflood at the external boundary, the behaviors of the ones presented in this paper are quite different at the boundary responses. And the effect of relevant parameters, including the dimensionless maximum water flux, the dimensionless beginning time of the water flux and the dimensionless external boundary radius, are analyzed on the production decline type curves. Finally, Blasingame type curves of a vertical well in water influx/waterflood reservoirs are verified by a field case study. This study can provide very meaningful references for reservoir engineers in water flux and the beginning time of the water flux evaluation by matching the type curves with actual field data.

References:

LE Doublet and T.A Blasingame. Decline Curve Analysis Using Type Curves:Water influx/Waterflood cases .SPE307741995.


Click here to agree
Poster 2 / 236

Productivity forecast model of vertical hydraulic fracturing well with varying conductivity in tight oil reservoir

Mingyu Cai1 ; Yuliang Su1 ; Yongmao Hao1 ; Wendong Wang1 ; Shiyuan Zhan1

1 School of Petroleum Engineering, China University of Petroleum (East China)

Corresponding Author(s): cmy9724@163.com

Hydraulic fracture has become an essential well stimulation technique in tight oil reservoirs. Large-scale vertical well fracturing can generate longer vertically oriented fractures to increase drainage area and, therefore enhance production and recovery efficiency of single well while also save costs1. The aim of this study is to develop a more practical productivity forecast model that can take into account of the heterogeneity of fracture distribution. Firstly, the fracture geometry model is established based on the features of pseudo three-dimensional model (P3D)[2] and the aperture changes along the length of hydraulic fracture. The hydraulic fracture is then divided into N segments. For each segment, fracture permeability is calculated by analyzing porosity change caused by proppant embedment, deformation, crush and diagenesis under the influence of effective closure pressure[3]. Finally, the productivity forecast model of vertically fractured well is established to deal with practical situations where the aperture and permeability of fractures cannot be neglected. The heterogeneous fracture model shows a good precision in the proof-test, and proved to be more credible and practicable than homogeneous model. We then report the results of several numerical simulations conducted for different values of fracture length, effective closure pressure and permeability of each segment, as well as a comparison with the simulated results of fracture model with homogeneity properties.

References:

Click here to agree

Parallel 8-B / 439

Proliferation rate estimation using a continuum-mechanical cancer cell model

Patrick Schröder1 ; Arndt Wagner2 ; Daniela Stöhr3 ; Markus Rehm4 ; Antje Jensch5 ; Nicole Radde5 ; Wolfgang Ehlers5

1 Institute of Applied Mechanics (CE), University of Stuttgart
2 University of Stuttgart
3 University of Stuttgart, Institute of Cell Biology and Immunology
4 Institute of Cell Biology and Immunology, University of Stuttgart
5 Institute for Systems Theory and Automatic Control, University of Stuttgart

Corresponding Author(s): patrick.schroeder@mechbau.uni-stuttgart.de

Once lung-cancer cells have invaded the brain tissue via the blood-vessel system, the cells proliferate and migrate in the tissue. The nutrients in the interstitial fluid ensure the proliferation and the
basal reactions of the cancer cells. Over time, the cancer cells proliferate and form metastases. In experiments, multicellular lung-cancer spheroids are grown under fully-nutrient-supplied conditions, which allow the comparison of the experiment to the early stage of the formation of lung-cancer metastases in a continuum-mechanical model. Moreover, the experiments enable the adaptation of relevant model parameters via maximum likelihood estimation.

In this contribution, the model is focused on the cancer-cell proliferation starting from an initial cancer cell amount within the tissue. Furthermore, the cells can spread within the brain tissue and, thus, increase the affected region. As a consequence of the time series of the experimental data, the model is simulated for the same observation period, allowing for the comparison of the overall cancer-cell amount in space and time.

In this contribution, the continuum-mechanical model is based on the Theory of Porous Media (TPM). Therein, the microscopic structure is volumetrically homogenised over a representative elementary volume leading to a macroscopic multi-phase model with interacting continua. In particular, the constituents are given by an elastic solid skeleton (brain cells) and two immiscible pore liquids (blood and interstitial fluid). Herein, the latter is a real mixture of the proliferating cancer cells and nutrients. The proliferation and consumption themselves are described via mass-production terms.

Numerically, the weak forms of the overall momentum balance and the adapted mass-balance relations are solved for their related primary variables. Thereby, the primary variables are the solid deformation, the pressures of the liquids as well as the concentrations of the cancer cells and the nutrients. The resulting coupled system of equations is solved monolithically applying the finite-element tool PANDAS. In this procedure, the spatial discretisation is realised via Taylor-Hood elements and the time is resolved on the basis of an Euler time-integration scheme.

Finally, the results are compared to the volumetric lung-cancer-cell data obtained from experiments. Thereby, an optimisation of the proliferation parameters is performed using the maximum likelihood estimation. This procedure leads to repeated executions of the numerical model and consequently to a better estimation of the proliferation rates.

References:

Parallel 9-E / 346

Propagation of fronts for Richards equation with gravity for general non-equilibrium capillarity pressure conditions

Hans van Duijn¹ ; Koondanibha Mitra¹ ; Sorin Pop²

¹ Eindhoven University of Technology
² Hasselt University

Corresponding Author(s): k.mitra@tue.nl

The Richards equation is a commonly used model for unsaturated flow through porous media. Using the Darcy law in the mass balance equation, and bringing the resulting equation to a dimensionless form, for gravity driven flow one gets the equation:
\begin{equation}
\partial_t S = \nabla \cdot \left[ k(S) \left( \frac{\nabla p}{\rho g} \right) \right],
\end{equation}

Here $N_c$ is the capillary number and $k(S)$ is a nonlinear function that is determined based on experiments. Two unknowns are involved: $S$, the water saturation and $p$, the water pressure. Standard models assume that these are related by a nonlinear relationship determined, again, based on experiments:
\begin{equation}
\begin{align*}
\gamma &= \frac{P}{S}, \\
\Delta \gamma &= \frac{P}{S} - \frac{P_0}{S}, \\
\end{align*}
\end{equation}

However, models based on this assumption cannot explain phenomena like saturation overshoot or finger formation, which are observed experimentally but ruled out as solutions to the standard Richards equation [DiCarlo (2004), Hassanizadeh & Gray (1993)]. Also, history dependent effects are disregarded [Morrow & Harris (1964)].

In this work we consider non-standard models, where dynamic and hysteretic effects are included in the $p$-$S$ relationship:
\begin{equation}
\begin{align*}
\gamma &= \frac{P}{S} - \frac{P^\alpha}{S} \mathbf{m} \mathbf{a} \mathbf{t} \mathbf{h} \mathbf{r} \mathbf{m} \{ \text{sign}(\partial_{\partial S} f(S) - \tau f(S)) \}, \\
\end{align*}
\end{equation}

To understand the behavior of this system in the one-dimensional case, we consider travelling wave (TW) solutions [van Duijn et al. (2017)]. We obtain the existence of TW and discuss their qualitative behavior. At first, the effects of capillary hysteresis and dynamic capillarity are considered separately. Then their combined effects on the general behavior of the system is delineated. These resulting solutions exhibit non monotone profiles and saturation overshoots, which is in good agreement with the experiments [DiCarlo (2004)].

Conditions for having saturation overshoots and reaching full saturation are derived and an extension to the existing model is proposed that includes the effect of non-vertical scanning curves. Finally, we present a numerical scheme to solve this mathematical model, discuss its convergence, and present some numerical results validating the theoretical findings.

References:


Click here to agree

Parallel 3-E / 194

Properties of Water Confined in Periodic Mesoporous Organosilicas: Nanoimprinting the Local Structure

Michael Fröba¹ ; Benedikt Mietner¹ ; Young Joo Lee¹ ; Felix Brieler¹

¹ University of Hamburg

Corresponding Author(s): froeba@chemie.uni-hamburg.de

The confinement of liquids in porous media greatly influences their physical properties, in particular, when the pore size approaches the molecular length scale. Several mechanisms, such as the pure geometrical restriction and the liquid-solid interaction at the interface contribute to the confinement effects, however, their roles for the drastic changes in the thermodynamic and dynamic behaviors of the liquids are not clearly understood. Especially, water molecules adsorbed on the surface and restricted within the pores are interesting in the scope of biochemistry, catalysis, and energy storage. The influence of the pore size on the melting and freezing points of confined water has been studied extensively. In contrast, fewer studies have been made concerning the effects of the surface polarity on the properties of spatially confined water, which may be due to the lack of highly defined porous substances. Periodic mesoporous organosilicas (PMOs) fill this gap perfectly because they combine the highly ordered pore structure of the well-established M41S-phases with the variety of surface chemistry within the pores. PMOs are synthesized using bis-silylated precursors
of the form (R’O)3Si-R-Si(OR’)3 where R is an organic bridging group which can be altered according to the desired surface properties. Furthermore, PMOs with an aromatic bridging group may exhibit a molecular-scale periodicity within the pore walls. This allows a periodically alternating surface chemistry along the pore channel, caused by arrays of silica and aromatic organic groups. It is assumed that water will adsorb differently at the diverse areas of the pore wall surfaces owing to the varying hydrophilic or hydrophobic properties. Because of the endless possibilities for the organic bridging function, the surface chemistry of PMOs can be fine-tuned. For example, when going from a benzene bridging group to a biphenyl bridge, the organic hydrocarbon part becomes larger and thus the overall pore wall becomes more hydrophobic. For a divinylalanine bridge, the amino function offers the possibility of forming hydrogen bonds with water, thus making the material considerably more hydrophilic. Here, we show that the molecular mobility of water confined in periodic mesoporous organosilicas (PMOs) is influenced by the polarity of the organic moiety. Multidimensional solid-state NMR spectroscopy directly probes the spatial arrangement of water inside the pores, showing that water interacts either with only the silicate layer or with both silicate and organic layers depending on the alternating surface polarity. A modulated and a uniform pore filling mode are proposed for different types of PMOs [2]. Our study gives a molecular-level picture of the adsorbate-surface interaction, which helps understanding various confinement effects and provides a new design concept of the pore structures with the desired properties.

References:

Click here to agree

Poster 1 / 599
Proppant embeded in shale during exposure to hydraulic fracturing fluids
Sarah Brown1; Johnathan Moore2; Dustin Crandall3; Alexandra Hakala3; Christina Lopano3; Wei Xiong4

1 AECOM at NETL
2 AECOM
3 NETL
4 ORISE, NETL

Corresponding Author(s): sarah.brown@netl.doe.gov

Proppants are small, granular additives used in hydraulic fracturing to keep induced fractures open and permeable after the reservoir pressure is lowered; typically sand is used. These materials are designed to resist the closure force across a fracture face and allow fluid to migrate out of the system. While the simple mechanical support of the proppant keeping a fracture open is well understood, the interplay between hydraulic fracturing additives, rock strength, and proppants is still lacking. Experiments were conducted on Marcellus Shale samples that were cored and saw cut to create an artificial, uniform fracture. 40/70 US Silica White™ proppant was loaded into the fracture. Cores were then subjected to a confining pressure of 20.7 MPa at a temperature of 71°C. Each core was then exposed to either deionized water, simulated hydraulic fracturing fluids, or air and allow to react for a period of 5 days. Each core was scanned using computed tomography (CT) before and after the test to evaluate for proppant embedment. Scanning Electron Microscopy (SEM) was used to take high resolution images of the fracture surfaces after the experiment to evaluate embedment features that occur below the CT scan resolution. Fractured cores that were filled with air or water did not exhibit mechanical signs of change in the CT or SEM. Rock integrity was not compromised and the proppants performed as designed with very little in the way of crushed proppant or rock material. When the hydraulic fracturing components were added, there were clear signs of indentation on the fracture surface.
Invited 4 (Room C) - Birol Dindoruk / 1116

Quantification of Multi-Scale Nature of the Porous Media Flows and Scale Up: Experimental and Numerical Challenges

Birol Dindoruk¹

¹ Shell Int. E&P

Corresponding Author(s): birol.dindoruk@shell.com

Fluid flow in porous media has attracted enormous attention from academia and industry as it has numerous applications, such as hydrocarbon production, shale gas recovery, CO2 sequestration and ground water utilization, etc. The fluid flow is governed by different phenomena at different scales ranging up to 12 orders of magnitude in dimension (nm to 100 m), from nanoscale (pore proximity), to microscale (wettability, contact angle, etc.), to core-scale (capillary pressure, relative permeability, etc.), and to reservoir-scale (geological heterogeneity, saturation distribution, vertical equilibrium, etc.). It is still challenging to describe the representative fluid flow properties with quantification at a single or few scales. For example, some of the challenges include the difficulty of simulating the rock-fluid interactions at pore level, the limitation of current imaging technologies in terms of incapability of characterizing the sub-micron pores, and the improper use of core-flood results (e.g., relative permeability, capillary pressure) in reservoir simulations without careful upscaling. This talk aims to cover the current state-of-the-art technologies for experimentation and simulation of multiphase fluid flow in porous media, and to shed light on some of the common pitfalls and drawbacks. Finally, this talk will also review some of the insights gained from previous studies by the industry regarding fluid behaviors that affect flow in reservoir rocks in terms of the following focus areas:
1) Containment, porous media: geometry, topology, connectivity, etc.
2) Fluids contained, multi-component, multi-phase
3) Containment (porous media)-Fluid interactions
4) Multi-Physics/Multiscale Natura of the transport

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 168

Quantifying Dual Porosity Flow and Contaminant Transport Processes Using an Integrated Pore-Scale Network Modeling Approach

Elizabeth May Ponte deiro¹ ; William Godoy² ; Fernanda Hoerlle² ; Martinus van Genuchten¹ ; Enno de Vries¹ ; Amir Raoo³

¹ Department of Earth Sciences, Utrecht University, Netherlands
² Department of Civil Engineering, LRAF, Federal University of Rio de Janeiro, Brazil
³ Department of Earth Sciences, Utrecht University, Utrecht, Netherlands,

Corresponding Author(s): e.t.devries@uu.nl
Many tropic soils exhibit double- or even triple-porosity features as reflected by heterogeneous pore- and/or particle-size distributions. While the amount of clay in tropical soils is generally relatively high, cementation of the finer particles into larger grains make field soil often behave macroscopically more like coarse-textured media. Natural aggregation may further enhance preferential flow paths for water and contaminant transport. The same can be observed in some sedimentary rocks (coquinas) composed partially or entirely of transported, abraded and/or mechanically-sorted fragments of the shells of mollusks, trilobites, brachiopods or other invertebrates. Such coquinas often contain large interconnected pore networks that directly or indirectly influence fluid flow and contaminant transport processes. Analysis of their pore properties (such as their size, shape and connectivity) as estimated from three-dimensional images (3D) provides a way to link microscale pore structures with their macroscopic functioning, and how all this may affect overall fluid flow processes in such media. We evaluated the applicability of an integrated characterization approach involving 3D microtomography, measurements of the pore-size distribution (PSD) using 3D images of two tropical soils, evaluating the double porosity nature of undisturbed soil samples, and modelling flow and transport using the PoreFlow pore network model. The procedure combines the use of commercial software such as Avizo, with in-house software developed at Utrecht University (Netherlands) and the University of Rio de Janeiro (Brazil). Images were obtained with a benchtop X-ray microtomography system at spatial resolutions of 3.6, 6, 12, and 30 microns by varying the size of the samples from 0.5 cm to about 4 cm in diameter. Pore-size distributions obtained at each image resolution were fitted with lognormal distribution functions. Results showed that large pore sizes are better represented in low resolution images of relatively large samples, while proper characterization of the smaller pores require higher resolutions of by necessity smaller samples. We also analyzed the PSDs obtained after skeletonization of the samples having different sizes. The image-based approach was found to correlate well with PSDs measured using mercury intrusion porosimetry. Saturated hydraulic conductivity estimates obtained with the pore network model were further compared with theoretical values based on soil texture.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-A / 283

Quantitative study of reservoir quality changes due to methane hydrate formation

Sulav Dhakal\textsuperscript{1} ; Ipsita Gupta\textsuperscript{1}

\textsuperscript{1} Louisiana State University

Corresponding Author(s): sdhaka5@lsu.edu

Subsurface methane hydrates have long been regarded as a potential energy source to power the future. Significant research efforts have been dedicated towards the exploration of methane hydrate reserves around the world. This study is focused on quantifying the diagenetic changes that occur during and after the formation of methane hydrates in the subsurface. A 2-dimensional geological model representative of the Gulf of Mexico subsurface stratigraphy has been prepared. Numerical simulation has been done using TOUGH+HYDRATE, a code developed at Lawrence Berkeley National Laboratory for modeling of hydrate bearing sediments using Integrated Finite Difference Method. Flow of thermogenic methane gas formed at a high pressure and temperature was simulated through a normal fault with shale and sandstone layers on top of each other. Preliminary results from the model is used as the representative of the hydrate formation phenomenon. Changes in the pressure, temperature, saturation of phases and permeability of the system is mapped in order to characterize the reservoir. As the rock and fluid flow properties are altered, the rate, location and shape and size of the hydrate formation changes. As the hydrates accumulate in the pores of the reservoir, the permeability of the hydrate zone decreases due to the clogging of the pores by solid hydrates. Inclusion of impermeable boundaries also determine the accumulation pattern and size of the hydrate formation.

References:
Parallel 5-D / 585

Quantum-computational approach to discrete tomography for porous media

Daniel O’Malley¹

¹ Los Alamos National Laboratory

Corresponding Author(s): oalled@lanl.gov

Making predictions about flow and transport in a porous medium requires knowledge of the heterogeneous properties of the porous medium such as permeability. Computational methods for inverse analysis are commonly used to infer these properties from quantities that are more readily observable (such as hydraulic head in a hydrologic context). We present a method for computational inverse analysis that utilizes a type of quantum computer called a quantum annealer. While quantum computing is in an early stage compared to classical computing, we demonstrate that it is sufficiently developed that it can be used to segment a porous medium into regions of high and low permeability. We utilize a D-Wave 2X quantum annealer to solve 1D and 2D inverse problems that, while small by modern standards, are similar in size and sometimes larger than similar inverse problems that were solved with early classical computers. Our results and the rapid progress being made with quantum computing hardware indicate that the era of quantum-computation in porous media may not be too far in the future.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 96

Quasi-static pore network modeling, revisited: a pore scale data-driven approach to investigate simulation correctness

Tom Bultreys¹; Qingyang Lin¹; Ying Gao²; Ali Q. Raeini²; Ahmed AlRatrou1; Branko Bijeljic¹; Martin J. Blunt¹

¹ Imperial College London
² Imperial College

Corresponding Author(s): t.bultreys@imperial.ac.uk

While quasi-static pore network models (PNM) have been used to investigate the relative permeability (Kr) behaviour of reservoir rocks since the seminal work by Bakke and Øren (1997), the capacity of these models to capture the appropriate physics and predict experimental data remains contentious (Sorbie and Skauge, 2011; Bondino et al., 2012; Berg et al., 2016). It is generally accepted that PNM have to be calibrated against relatively cheap experimental data in order to predict more complex experiments. However, even after matching the former, it is not clear when and why PNM fail to reproduce experimental trends in the latter. We propose that the main reason for this is that the information in the Pc and Kr-curves is extremely densely encoded: many aspects of the porous medium and the fluid behaviour are lumped into the same parameter. PNM are thus very likely overfitted, making it hard to assess whether model failure is due to inappropriately trained model parameters or due to a fundamentally lacking description of the pore scale flow physics.
To unravel this, there is a need for experimental data which probes the underlying properties that make up a Kr-curve. Thanks to recent innovations in micro-computed tomography (micro-CT), it is now possible to image a rock’s pore scale fluid distribution during flow experiments. We propose that this data can be used to constrain the source of errors in a PNM, if the issue is addressed by investigating three questions in specific order (by decreasing fundamentality):

1. Does the model predict the correct pore scale fluid distributions? This relies on the accuracy of the pore and throat radii, on the assigned contact angles in each pore and throat, and on the physics implemented in the invasion algorithm.

2. Does the model predict the correct saturation for a certain fluid distribution? This depends on the volume partitioning between pores and throats and thus on pore/throat length partitioning, which is arbitrary; as well as on the description of wetting layers.

3. Does the model predict the correct flow rate for a certain fluid distribution? This is chiefly determined by calculation of the pore, throat and layer conductivity in the model.

In this work, we focus on the first question. We present a novel modeling/experimental methodology to compare the pore-by-pore fluid distributions in a PNM to micro-CT based steady-state flow experiments. Using this analysis, we assess the importance of errors in the filling state of pores and throats to the flow, while seeking to split off the influence of volume and conductivity assignment. The influence of the pore scale contact angle distribution is investigated by automatically measuring a large number of contact angles on an in-situ micro-CT image (AlRatout et al., 2017). Each of these contact angles is assigned to the pore that corresponds with its location in the image. This allows to perform PNM simulations with directly measured contact angle distributions for the first time. We explore how this influences PNM simulation errors by comparison to simulations with contact angles drawn from random distributions. The correctness of an adapted version of the FNM approach outlined in Dong (2007) and Valvatne and Blunt (2004) is investigated by applying the methodology to a water-wet Bentheimer sandstone. In drainage, the model is found to reproduce the main oil flow paths in the experiment, while however significantly overestimating the corresponding water saturation. In imbibition, tentative results show a higher level of snap-off in the experiment compared to the model.

Acknowledgements:
Steffen Berg and Øve Wilson (Shell) are thanked for valuable comments and discussions on this work. Shell is acknowledged for financial support and for permission to present this abstract.

References:


Click here to agree

Parallel 8-G / 386

Quaternions Formulation of Linear Thermoporoelasticity
Mario-Cesar Suarez-Arriaga

1 International Geothermal Association - Asociacion Geotermica Mexicana

**Corresponding Author(s):** mcsa50@gmail.com

This paper introduces an original application of the hypercomplex numbers known as Quaternions to model non-isothermal processes in porous rocks. The general thermoporoelastic linear theory is introduced in four dimensions and reformulated as a set of quaternions. The need of the fourth dimension appears naturally because of the pores presence. It is shown that a minimum set of four independent experimental coefficients are necessary for the coupling of four strain tensors: two for the bulk porous medium, one for the fluid and one for the total thermal expansion. Once a basic set of parameters are defined, any other coefficient can be deduced algebraically. This formulation could become a new mathematical tool to represent thermoporoelastic phenomena because it includes both, the fluid pressure changes and the temperature changes.

**References:**


Click here to agree

**Parallel 8-H / 613**

**RBF-FD approximations based on polyharmonic splines basis with supplementary polynomials applied in a pore-scale problem**

Luis Guilherme Cunha Santos1 ; Eduardo Abreu2

1 Unicamp

2 University of Campinas, Sao Paulo, Brazil

**Corresponding Author(s):** lgcunhas@yahoo.com.br

The Radial Basis Function generated Finite Differential (RBF-FD) is a meshless method that has attracted attention in the last decades by its flexibility in the numerical approximation of PDEs, simplicity of computational implementation and ease in the approach of complex geometries. It has already been successfully applied to various engineering problems such as heat transfer, electrostatics, vibration, seismic modeling, and in particular, fluid dynamics problems [1, 2, 3, 4, 5]. In this way, RBF-FD is a good candidate in a range of increasing applications of numerical simulations including seismic exploration of oil and gas, among others [6]. In this work, we present applications of RBF-FD with polyharmonic splines basis (PHS) with supplementary polynomials, RBF(PHS)-FD for short, in two benchmarks using the vorticity and stream-function formulation: i) problem of natural convection of air in a square cavity for some values of Rayleigh number; ii) problem of driven flow in a square cavity for several Reynolds number values. In both problems, we discretize the domain in uniform point clouds and non-uniform point cloud. Finally, after the validation of the benchmark results, the RBF (PHS)-FD is applied and discussed for a problem of flow of a fluid in the pore scale with a complex geometry. We will also add some comments about the use of multiscale meshless method for porous media transport problems.

**References:**


Click here to agree

Poster 2 / 876

ROCK ABSOLUTE PERMEABILITY ANALYSIS USING IMAGE-BASED DIRECT PORE-SCALE SIMULATIONS

Clément Varloteaux\(^1\); Igor Bondino\(^2\); Igor Bogdanov\(^3\)

\(^1\) CHLOE  
\(^2\) Total  
\(^3\) laboratoire CHLOE, Université de Pau

Corresponding Author(s): clement.varloteaux@univ-pau.fr

The direct numerical simulations (DNS) experience of pore-scale flow is still relatively scarce and laborious due to the numerous practical challenges. They include typically huge model size and high computational expenses, some uncertainties in geometrical description related to resolution size and other factors remaining much in common for single and multiphase flow cases. Sometimes this makes challenging an unambiguous definition of rock permeability based on numerical simulations.

The advantage of DNS comprises the ability to model in detail dynamic physical fields interaction in “real” pore volume (and/or solid matrix) geometry. In our current work we address the incompressible steady single-phase flow in voxel-based geometry of 3D real rock image (more precisely, stack of images) with the main objectives to analyze and quantify the impact of image processing workflow on permeability computation.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 4-C / 349

Reactive Alteration of Rough-Walled Fractures in Gradient and Kinetic Regimes with Applications
Flow and transport processes in fractured rock are strongly influenced by fracture aperture and diffusive interactions between the fractures and rock matrix. The transmissivity of fractures is highly sensitive to fracture aperture (a cubic dependence). Complex thermo-hydrologic-mechanical (T-H-M-C) coupled processes that alter fracture apertures thus drive feedbacks and pattern formation. For example, dissolution of fracture surfaces increases their aperture and transmissivity, whereas precipitation has the opposite effect. We adopt aperture-integrated approaches for modeling fracture alteration and the resulting evolution of flow, concentration, temperature and aperture fields. I will present examples from previous and ongoing research on fundamental aspects of fluid flow, reactive transport and coupled processes in fractured rock, including comparisons to controlled high-resolution experiments. Behavior in both kinetic regimes (where disequilibrium drives water-rock interaction) and gradient reaction regimes (where solubility gradients drive dissolution-precipitation) are considered. Dissolution of fracture walls by reactive solutions produces highly preferential aperture growth, either by unstable finger propagation in the kinetic regime, or by selective growth in the gradient reaction regime. These phenomena are relevant in the context of acid injection for permeability enhancement in energy recovery systems, water-rock interactions during geological CO2 sequestration, and natural phenomena such as karst and cave formation. Precipitation reactions lead to unusual growth of elongate precipitate bodies perpendicular to the mean flow direction. We also present results from geological scale mountain-hydrologic systems with thermo-hydro-chemical coupling relevant to the formation of hypogene or thermal karst systems. In these systems, both the temperature-dependent (retrograde) solubility of calcite, onset of buoyant convection after a threshold Rayleigh number is reached due to the growth of fracture transmissivity by dissolution, influence the growth patterns that result. Recent applications of our modeling approach to thermo-hydro-chemical coupling in geothermal energy doublet-flow systems reveals useful strategies for sustaining energy production. In silica-dominated geothermal energy reservoirs, we show that injection of undersaturated water leads to long-term sustainable operation of the system. We also show that after an initial period of 1-2 years, sustained energy extraction can be sustained even with recirculation, because silica concentrations do not build up in recirculated water. The large difference in solute versus thermal diffusivity of the rock matrix, however, ensures that thermal energy recovery is sustained. With oversaturated injection, a band of precipitation forms at some distance from the injection well, encapsulating the flow system and limiting heat recovery.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 362

Reactive Transport Modelling on the Drill Core Scale, Parameterized by GeoPET/μCT Process Tomography

Johannes Kulenkampff1; Lotfollah Karimzadeh1; Stefan Schymura1; Sebastian Eichelbaum2; Johanna Lippmann-Pipke1; Cornelius Fischer1

1 HZDR
2 nemtis
3 BGR

Corresponding Author(s): c.fischer@hzdr.de

In-situ leaching of ores is considered as an economic and environmentally friendly production method. However, the leaching process is complicated by its dependence on the material’s heterogeneity and
by retroactive effects over large scales. We developed an experimental procedure which is based on positron emission tomography (PET) during transport experiments with radiotracers (Kulenkampff et al. 2016), supported by µCT, to derive flow and diffusion parameters with molecular sensitivity (picomolar) and with reasonable resolution (1 mm) on samples with drill core dimensions. The procedure directly yields the spatial distributions of flow velocity and effective volume from flow experiments, the diffusion coefficient, and the real geometry of the sample. This approach is validated by using a core sample (L = 10 cm, D = 6 cm) with an induced fracture, obtained from Permain Kupferschiefer sandstone. After the tomographic measurements the core sample was leached step-wise with (1) fresh water to remove salt minerals, (2) acidic solution (H2SO4, pH 1.5) to reduce the carbonate content, and (3) acidic solution with added ferric iron to dissolve the Cu-sulfidic ore.

The measured hydrodynamic and structural parameters from PET and µCT were then directly imported into a reactive transport model using interface Comsol Multiphysics with Phreeqc (iCP, Nardi et al. 2014) to simulate core sample leaching. The geochemical conditions of the simulation were considered consistent to the laboratory leaching experiment. The reactive transport simulation is based on the real geometry of the sample and the observed flow fields on the continuum scale and does not require a high performance computation of flow simulations on pore scale. The results of these economical simulations are compared to the results of the laboratory leaching experiments.

References
J. Kulenkampff, M. Gründig, A. Zakhnini and J. Lippmann-Pipke. Geoscientific process monitoring with positron emission tomography (GeoPET), Solid Earth, 7, 1217-1231, (2016).

References:
Acceptance of Terms and Conditions:
Click here to agree

Invited 2 (Room A) - Anne De Wit / 1120

Reactive fingering instabilities in CO2 sequestration
Anne De Wit1

1 Universite libre de Bruxelles (ULB)

Corresponding Author(s): adewit@ulb.ac.be

To decrease the atmospheric concentration of CO2, sequestration techniques whereby this greenhouse gas is injected in saline aquifers present in soils are considered. Upon contact with the aquifer, the CO2 can dissolve in it and subsequently be mineralized via reactions with minerals like carbonates for instance. We investigate experimentally the influence of such reactions on the convective dissolution of CO2 by analyzing convective density fingering patterns developing when gaseous CO2 is put in contact with aqueous solutions of reactants in a confined vertical geometry. We show that the reactions can enhance convection inducing a more efficient sequestration [1,2]. In parallel, we also analyze precipitation fingering patterns obtained when a solution of carbonate is injected into an aqueous solution of calcium ions. We show that the amount and spatio-temporal distribution of the solid calcium carbonate phase produced strongly depends on the concentrations and injection flow rate [3,4,5]. Emphasis will be put on the possibility to control the convective and precipitation fingering pattern properties by varying the very nature of the chemicals or injection conditions. Implications on the choice of optimal sequestration sites will be discussed.

References:
Parallel 9-E / 440

Reconstruction of complex 3D pore structure in carbonates from 2D images using global optimization

Author(s): Tianshen Huang
Co-author(s): Zeyun Jiang 1; Rink van Dijke 1; Sebastian Geiger 1; Dmytro Petrovskyy 1

1 Heriot-Watt University

Accurate characterization of the multiscale pore structure in carbonates reservoirs is a complex but crucial step for pore-scale modelling of the corresponding flow and transport properties. 3D images obtained using micro computed tomography (CT) are only able to capture a relatively narrow range of pore sizes at a given resolution and fail to reproduce cross-scale pore connections. Therefore, reconstruction of 3D models of pore structures based on widely available large high quality 2D images (e.g. SEM) is an attractive alternative. In this study we introduce an Expectation-Maximization global optimization algorithm, inspired by the field of texture synthesis, to generate 3D models from 2D training images (TIs), preferably in different directions. The method is developed for not only granular media, but also more general porous media, in particular carbonates. The core idea is an iterative refinement of orthogonal patterns for every voxel, which alternates between finding the best matching local patterns from the TI for every voxel (Expectation step) and minimizing the global difference between the best matching and reconstruction patterns (Maximization step). This iterative algorithm preserves much better the continuity of pore and solid structures in all three directions than conventional pixel or pattern based methods. Additionally, we introduce a distance map transformation for both the pore and the solid phases in the binary TIs to enrich their spatial distributions. This enables us to model complex structures with highly variable pore and solid sizes. Furthermore, we identified that the principle component analysis (PCA), which is normally used to reduce computational complexity, results in a significant loss of pore connectivity in the 3D reconstructions. Instead, we have introduced an adapted k-coherence search algorithm, which not only prevents the loss of connectivity, but also reduces the nearest pattern search (Expectation step) complexity to constant time (compared to conventional logarithmic time). Moreover, the core iterative algorithm can be parallelized through multi-thread CPU and can easily be adapted to GPU, hence the computational efficiency of our method is much improved. Our comprehensive tests show that the reconstructed models (e.g. Fig. 1) correctly capture the complex geometrical features (e.g. pore shape, long pore channels and wide range of pore sizes as well as the topology, particularly the connectivity between small and large pores), which is reflected in accurate simulation of single- and two-phase flow properties.
Figure 1: enter image description here

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-D / 646

Recovery of Non-Aqueous Phase Liquids (NAPL) from porous media using food grade amphiphiles.

Chike Ezeb 1, Chia-Yu Chen 1, Kyriakos Papadopoulos 1

1 Tulane University
Corresponding Author(s): cezeh@tulane.edu

Food-grade surfactants Lecithin (from soy) and Tween 80 (used in food such as ice-cream) were employed for the mobilization of non-aqueous-phase liquids from porous media. The hypothesis of this work was that food grade surfactants can be employed for oil-spill remediation and that there may be a synergistic benefit when two surfactants are combined. The non-aqueous phase of this project was Hexadecane (red dye was added to improve visualization), and the aqueous phase consisted of different ratios of the surfactants Lecithin and Tween 80. From the study, it was determined that a 40:60 by weight Lecithin-Tween 80 mixture has a better performance in the mobilization of Hexadecane from the porous medium than either surfactant at the same overall surfactant concentration. This study was exploratory and warrants further research in the realm of EOR (Enhanced Oil Recovery) and OSR (Oil Spill Remediation).

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-H / 373

Recursive Parallel Implementation of Multiscale Mixed Methods

Eduardo Abreu¹ ; Paola Ferraz² ; Het Mankad³ ; Felipe Pereira⁴ ; Fabrício Sousa⁵

¹ University of Campinas, Sao Paulo, Brazil
² University of Campinas, Sao Paulo, Brazil.
³ The University of Texas at Dallas
⁴ Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA
⁵ University of Sao Paulo

Corresponding Author(s): pferraz@ime.unicamp.br

We are interested in the numerical approximation of partial differential equations of elliptic nature, in the context of incompressible two-phase flow problems in heterogeneous porous media. Numerical solutions of elliptic boundary value problems with high contrast and discontinuous coefficients are often expensive and time consuming, so efficient numerical methods are necessary. Indeed, methods that can take advantage of CPU-GPU clusters are of particular interest because GPUs have larger computational power than CPUs alone. In this work, we focus on the multiscale mixed method MuMM introduced in [1] (see also [2] where the variational formulation of [1] was presented), that is based on a non-overlapping iterative domain decomposition procedure with Robin interface conditions. Local multiscale basis functions are calculated in each subdomain to represent the discrete solutions that can be efficiently computed in CPU-GPU clusters. The method presented here uses a new technique to cluster multiscale basis functions associated with nearest neighbor subdomains, leading to a small (and local) linear system for the interface between the subdomains. The global solution is obtained by recursively applying the MuMM to all pairs of subdomains until the union of subdomains reach the whole domain. The resulting interface linear systems are easily handled by Schur decomposition along with a LU factorization. The novelty of this method is that it does not use an iterative procedure to compute the global solution and shows excellent parallel performance. Numerical experiments related to benchmark problems in petroleum engineering will be presented and discussed.


References:


Click here to agree

Parallel 8-C / 94

Reduced Models of Flow and Mechanics in Fractured Porous Media

Author(s): Jan Stebel

Co-author(s): Jan Březina

1 Technical University of Liberec

Corresponding Author(s): jan.stebel@tul.cz

We present a mathematical model of flow and solid mechanics in saturated fractured porous media based on the Biot poroelasticity. The fractures are treated as lower-dimensional manifolds on which the system of equations is projected onto the tangent space and coupled to the surrounding through interface conditions. The model can describe porous fractures, fractures filled only by a liquid and a transition between these two states.

Several finite-element and discontinuous-Galerkin discretizations are introduced and their stability is studied on a model problem. We decouple the system of equations to the flow and mechanics part and to the fracture and the surrounding domain. The convergence of iterative splittings for the decoupled problem is compared to the monolithic approach.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-A / 107

Reduction of Interfacial Instabilities in Miscible Displacements in Subsurface Porous Media

Author(s): Qingwang Yuan

Co-author(s): Jinjie Wang

1 Stanford University

2 China University of Geoscience

Corresponding Author(s): qyuan@ucalgary.ca

In the present study, miscible displacements are investigated through nonlinear numerical simulations. A practical scenario with concentration-dependent diffusion and velocity-induced dispersion
is considered, which is widely encountered in many areas involving flow and transport in subsurface porous media. Different with most of previous studies with a constant injection rate, the time-dependent displacement rates are used in the present research with the same amount of fluid injected. Under the scenario when dispersion is considered, the cycle period, amplitude and dispersion have a complex effect on the development of interfacial instabilities as well as mixing of two fluids. By varying period and amplitude, the displacements with either more unstable case with higher degree of mixing or less unstable case with larger sweep efficiency and later breakthrough time can be achieved, when compared with the widely used constant injection rate. The time-dependent rates therefore have either destabilizing or stabilizing effects on displacements depending on the values of them. This also indicates that the interfacial instabilities and mixing of miscible displacements can be controlled and optimized with the time-dependent rates.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 611

Refractive-light-transmission measurements of density-driven convection with application to solubility trapping of geologically sequestered CO2

Maria Rasmusson1 ; Fritjof Fagerlund1 ; Kristina Rasmusson1 ; Yvonne Tsang2 ; Auli Niemi1

1 Uppsala University
2 Lawrence Berkeley National Laboratory

Corresponding Author(s): auli.niemi@geo.uu.se

Density-driven convection can accelerate the rate of CO2 solubility trapping during geological CO2 storage in deep saline aquifers. We present a bench-scale experimental method based on refractive light transmission (RLT) in an analogue system that enables comprehensive study of solutally induced density-driven convection in saturated porous media. In an analogue system, we investigate density-driven convective mixing under conditions relevant to geological CO2 storage. A range of Ra values relevant to potential storage sites are investigated by varying the grain size and density contrast in the laboratory setup. We show that the method accurately determines the solute concentration in the system with high spatial and temporal resolution. We can thereby quantify the onset time of convection (t_c), mass flux (F) and flow dynamics for the different Ra values tested. Based on our findings, we present a scaling law for t_c. The resulting dependence of t_c on Ra, indicates that t_c is more sensitive to large Ra than previously thought. Our findings can also show why F is described equally well by a Ra-dependent or a Ra-independent scaling law. The new method and findings can serve to improve the understanding of convective mixing processes in saturated porous media, and aid the assessment of CO2 solubility trapping, including potential for trapping under given field conditions.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 6-G / 427
Relations between seepage velocities in immiscible two-phase flow in porous media

Author(s): Alex Hansen

Co-author(s): Santanu Sinha  ; Dick Bedeaux  ; Signe Kjelstrup  ; Magnus Aa. Gjennestad  ; Morten Vassvik

1 NTNU
2 Norwegian University of Science and Technology
3 Norwegian University of Science and Technology, NTNU, Trondheim
4 Department of Physics, Norwegian University of Science and Technology

Corresponding Author(s): alex.hansen@ntnu.no

Based on the volumetric flow rate in immiscible two-phase flow in porous media under steady-state conditions*, being an Euler homogeneous function of order one, we have earlier derived a set of relations between velocities that describe the flow of the two immiscible fluids. These velocities we call thermodynamic velocities and they are distinct from the seepage velocity of each fluid. However, the two sets of velocities, the thermodynamic velocities and the seepage velocities, are related through a linear transformation. This transformation encodes the effect of the porous medium on the mixing of the immiscible fluids.

We use the theory on four analytically solvable variants of the parallel capillary tube model: 1) The capillaries are completely filled with either immiscible fluid; 2) the capillaries are filled with a mixture of each fluid; 3) a subset of the capillaries are so narrow that only the wetting fluid may enter whereas the rest of the capillaries are filled with either fluid, and 4) a subset of the capillaries are so narrow that only the wetting fluid may enter whereas the rest of the capillaries are filled with a mixture of the two immiscible fluids.

Lastly we analyze numerically a network model using our theory.

In all cases, we demonstrate the consistency of the models with the theory.

*By steady-state flow we mean that the macroscopic flow parameters fluctuate around well-defined averages in contrast to stationary flow where the microscopic interfaces remain fixed.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 292

Research on stress sensitivity of fractured carbonate reservoir by CT Technology and pore-scale simulation

Zhihui Liu  ; Yongfei Yang

1 China University of Petroleum (East China)

Corresponding Author(s): happy4615@163.com

Fractured geological formations are ubiquitous throughout the world, and their stress-sensitive behaviors are of primary interest in a number of contexts. In this study, a stress sensitivity experiment on carbonate core plugs in which micron Computed Tomography (μ-CT) technology is applied to visualize and quantitatively evaluate morphological changes to the fracture aperture with respect to confining pressure. Fracture models were obtained at selected confining pressures on which pore-scale flow simulations were performed to estimate the equivalent absolute permeability. The results showed that with the increase of confining pressure from 0 to 0.6 MPa, the fracture aperture and
equivalent permeability decreased at a greater gradient than their counterparts after 0.6 MPa. This meant that the rock sample was more stress-sensitive at low effective stress than at high effective stress. On the loading path, an exponential fitting was found to fit well between the effective confining pressure and the calculated permeability. On the unloading path, the relationship was found partially reversible, which can evidently be attributed to plastic deformation of the fracture as observed in CT images.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 22

**Researches on residual oil saturation and micro displacement mechanism after different oil displacement modes in tight oil reservoir**

**Author(s):** Ting Chen

**Co-author(s):** ZhengMing Yang ; YuTian Luo ; ShengChun Xiong ; Jiaxiang Xu

1 *University of Chinese Academy of Sciences*

2 *PetroChina Research Institute of Petroleum Exploration & Development*

3 *PetroChina Research Institute and Development Institute of Petroleum*

**Corresponding Author(s):** chenting15@mails.ucas.edu.cn

In view of the present situation of low productivity and the difficulty of water injection development in the tight reservoir. In order to improve the development effect of tight reservoir, select cores with different permeability grade parallel samples, and carried out injection of simulated formation water, active water, CO2 and N2 physical simulation experiment. Combined with nuclear magnetic resonance technology investigates micro pore structure of tight oil cores, mobile fluid saturation, recovery ratio and residual oil distribution for different pores. Investigation have shown that for tight oil reservoir, most of the pores are sub-micro pore and micro-nano pore, the movable fluid is mainly stored in the pores of more than 1μm. Micro pores and sub-micro pores contribute most of the produced oil. The effect of active water flooding is slightly better than water flooding and active water could effectively drive oil out of the micro-nano hole. CO2 and N2 flooding effects is obviously better than the effects of conventional water flooding and active water flooding, and they have relatively good oil displacement effects at micro pores and sub-micro pores. The higher the permeability is, the better the CO2 flooding effect is; the lower the permeability, the better the N2 flooding effect.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-E / 339

**Respective contributions of adsorption, surface and bulk confined diffusion in molecular transport in nanoporous materials**

Pierre Levitz

1 *CNRS*
**Corresponding Author(s):** pierre.levitz@upmc.fr

Numerous porous materials are made of intricate clustering of polydisperse nanoparticles. The particle organization on a length-scale ranging from nanometers to some micrometers is a cornerstone to properly understand transport properties (diffusion-permeation). A strong need to a bottom-up approach mixing SAXS, SANS and 2D-3D imagery technics is highly suitable for these types of multiscale complex systems. This multimodal structural analysis offers the possibility to use 3D reconstructions and to build constrained models mimicking observed geometrical features. These models can then be used to compute transport properties allowing comparison with experimental determinations.

In this talk, we focus on a long and slow dynamics inside nanoporous porous materials essentially driven by molecular diffusion. This mechanism plays a major role to estimate the sustainability over a long period of time of numerous manufactured porous materials. We analyze the interplay between pore structure, adsorption and diffusion and how these different processes act in long term molecular transport. We show how intermittent dynamics involving adsorption, surface diffusion and relocation inside the pore space induces a large part of the strong reduction of molecular diffusion inside pore network.

**References:**


**Acceptance of Terms and Conditions:**

Click here to agree

---

**Poster 4 / 121**

**Response of Relative Permeability to Coal Surface Chemistry through Steady-State Core Flooding Measurements using X-ray CT Scanner and Packed Bed Samples**

**Author(s):** Fabio Terzini Soares

**Co-author(s):** Lei Ge ; Thomas E. Rufford ; Karen Steel ; Sandra Rodrigues ; Victor Rudolph

1 The University of Queensland

**Corresponding Author(s):** f.terzini@uq.edu.au

The relative permeability behaviours of gas and water in coal are primary factors in the productivity of a coal seam gas reservoir, and it is dependent on many factors including fluid saturations and pressure, cleat geometry and network, and wettability (surface chemistry). In this study, we performed steady-state relative permeability measurements using X-ray CT scanner on packed beds of coal particles to allow systematic investigation of coal surface chemistry on permeability behaviour. Packed bed approach provides a homogeneous, isotropic coal sample with controllable coal surface properties; pore size and channel geometry (by control of particle size), and also removes the natural cleat geometry effects from the experimental measurement.

In this paper, we compare packed cores made with coals from two different locations within the Bowen Basin, Queensland, Australia. Both samples have the same rank (1% random reflectance), but with different maceral composition. The sample from Broadmeadow (BRDM) is vitrinite rich (76% mineral-matter free basis) and the sample from Isaac Plains (IP) is inertinite rich (61% mmib) – both petrographic and proximate analyses were carried out. Samples were constructed using coal particles with size between 53 – 212 μm, resulting in a packed bed with porosity around 19%.

Core flooding experiments were conducted at a constant effective pressure of 22 bar followed by a sensitivity analysis using a hypothetical coal seam gas reservoir simulation model. The CT images were used to calculate water saturation based on the grey-scale without relying on the dead-end volumes of the core flooding system. The relative permeability curves suggest that the vitrinite rich coal (BRDM) had a more water-wet behaviour than the inertinite rich coal (IP), where the crossover point occurs at (krw=krg=0.45; Sw = 0.62), for the BRDM, and at (krw=krg=0.32; Sw = 0.44) for the IP. Hypothetical simulation using Eclipse shows that the cumulative water production for the IP
can be 40% higher than the BRDM over a period of 30 years of gas production, due to its water wet behaviour.

References:


5. (a) Drellich, J.; Miller, J. D.; Good, R. J., The effect of drop (bubble) size on advancing and receding contact angles for heterogeneous and rough solid surfaces as observed with sessile-drop and captive-bubble techniques. J Colloid Interf Sci 1996, 179 (1), 37-50; (b) Li, Q. Z.; Lin, B. Q.; Zhao, S.; Dai, H. M., Surface physical properties and its effects on the wetting behaviors of respirable coal mine dust. Powder Technology 2013, 233, 137-145.


7. (a) Fuerstenau, D. W.; Diao, J., Characterization of Coal Oxidation and Coal Wetting Behavior by Film Flotation. Coal Preparation 1992, 10 (1-4), 1-17; (b) Fuerstenau, D. W.; Diao, J.; Williams, M. C., Characterization of the wettability of solid particles by film flotation 1. Experimental investigation. Colloid Surface 1991, 60 (0), 127-144.

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-G / 336

Risk Assessment of Carbon Sequestration into A Naturally Fractured Aquifer at Kevin Dome, Montana

Minh Nguyen1 ; Tsunasa Onishi2 ; Philip Stauffer3 ; Bill Carey4 ; Ye Zhang1

1 University of Wyoming
2 Texas A&M University
3 Los Alamos National Laboratory

Corresponding Author(s): bcarey@lanl.gov

As actual CO2 injection is unlikely to take place at Kevin Dome, Montana, the Big Sky Carbon Sequestration Partnership has turned to maximizing the value of existing data acquired at the site. We
present the risk assessment work done using the National Risk Assessment Partnership (NRAP) to Kevin Dome, Montana. Geologic CO2 sequestration in saline aquifers poses certain risks including CO2/brine leakage through wells or non-sealing faults into ground water or land surface. These risks are difficult to quantify due to data availability and uncertainty. One solution is running large numbers of numerical simulations on the primary CO2 injection reservoir, shallow reservoirs/aquifers, faults, and wells to assess leakage risks and uncertainties. However, a full-physics simulation is usually too computationally expensive. NRAP integrated assessment model (NRAP-IAM) uses reduced order models (ROMs) developed from numerical reservoir simulations of a primary CO2 injection reservoir to address this issue. A powerful stochastic framework allows NRAP-IAM to explore complex interactions among many uncertain variables and evaluate the likely performance of potential sequestration sites. In this study, we investigate the sensitivity of a variety of uncertain parameters to CO2/brine leakage through (1) legacy wellbore and (2) fault pathways. We found major uncertain parameters to which the potential CO2 leakage through legacy wellbore is sensitive including values of fracture permeability, end-point CO2 relative permeability, capillary pressure, and permeability of confining rocks. CO2 and brine leakage through fault pathways is sensitive to fracture permeability, length of the faults, and fault displacement.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-A / 458

Robust algorithms for stability analysis and flash calculation of reservoir fluids at constant moles, volume and temperature

Shuyu Sun¹

¹ King Abdullah University of Science and Technology (KAUST)

Corresponding Author(s): shuyu.sun@kaust.edu.sa

Accurate modeling and robust computation of the phase behavior is essential for optimal design and cost-effective operations in petroleum reservoirs as well as in petroleum processing plants, where we need to understand the fluid flow of partially miscible multi-component multi-phase mixture in free spaces or in porous media. Phase behavior calculation of fluid mixture consists of stability analysis and flash equilibrium calculation. The goal of the NVT stability analysis is to determine whether a phase is stable at specified volume, temperature, and mole numbers. If it is not stable, the NVT flash equilibrium calculation is to establish the composition and amount of each stable phase after phase splitting. Conventional algorithms for stability analysis and flash calculation are based on fixed-point iteration, Newton-type iteration, or their combination, and the convergence has never been guaranteed. In this work, we propose an energy-stable iterative method for NVT stability analysis and NVT flash equilibrium calculation. We consider fluid mixture modeled by the Peng-Robinson equation of state, and our proposed algorithm is an iterative algorithm motivated from the dynamics of two-phase fluid system with Fick’s law of diffusion for multi-component fluids. The proposed iterative procedure is proven to be energy stable under certain conditions. Numerical examples are tested to demonstrate efficiency and robustness of the proposed method. We also discuss the extension of the algorithm to NVT flash in multiple spatial dimensions, which can be used to model the interface of nonzero thickness between two phases.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 259
Robust level set methods for moving interfaces

Peter Frolkovic

1 Slovak University of Technology

Corresponding Author(s): peter.frolkovic@gmail.com

We present recent results relevant for an application of level set methods to track moving interfaces and free boundaries. We cover the most important tasks typically required in level set methods like an advection of level set function, a preservation of signed distance property, and an extrapolation of missing data in the normal direction to the interface.

Typically a movement of the interface is driven by some additional processes that require a coupled modelling on evolving domains. The level set methods result in implicitly defined computational domains when some interface conditions must be approximated without an explicit reconstruction of the interface. For that purpose the immersed interface methods are developed for convenient unfitted grids. The methods are well covered for elliptic and parabolic problems, but not so much for a hyperbolic type of problems. The reason is so called cut cell problem due to a CFL time step restriction for numerical schemes with an explicit in time discretization that are typical for hyperbolic problems. We are interested in semi-implicit methods that are unconditionally stable with respect to the choice of time steps and that have no CFL restriction for cut cells.

A brief illustration of the level set tools will be given for a flow in porous media with an evolving part of a boundary (a moving groundwater table).

References:


Click here to agree

Invited 4 (Room A) - Florin Adrian Radu / 1103

Robust numerical simulation of poromechanics

Florin Adrian Radu

1 University of Bergen

Corresponding Author(s): florin.radu@uib.no

In this work we consider robust iterative methods for the effective simulations of poromechanics, which has plenty of societal relevant applications like geothermal energy, CO₂ sequestration or oil recovery, to name a few. We will focus on the quasi-static linear Biot model and non-linear extensions.

We start with the well-recognized fixed stress method [1, 2] and present some recent convergence results for heterogeneous media [3] and higher order space-time elements [4]. Next, we introduce a new, parallel-in-time fixed stress scheme [5]. Further, we consider a non-linear extension of the Biot model and study different (monolithic or splitting) iterative schemes for it [6]. The linearization will be based on Newton’s method or a variant of it, the L-scheme, see e.g. [7]. Finally, we move to unsaturated/saturated flow and poromechanics. Now, also the coupling flow-mechanics term is non-linear, which makes the problem even more challenging. A fixed stress type method, combined with the Newton or L-scheme will be presented. Anderson acceleration will be used. Especially, we will show the general ability of the Anderson acceleration to effectively accelerate convergence and
stabilize the underlying scheme, allowing even non-contractive fixed-point iterations to converge [8]. Both rigorous convergence results and illustrative numerical examples will be presented.

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 873

Rock-Based, 2.5D Ceramic Micromodels

Daniel Park¹; J. Upadhyay¹; Khurshida Sharmín²; J. Robbins¹; I. Schoegl¹; Karsten ThompsonNone; Dimitris Nikitopoulos³

¹ Louisiana State University
² Dhaka University of Engineering & Technology
³ Louisiana State University, Mechanical and Industrial Engineering Department

Corresponding Author(s): medimi@lsu.edu

Micromodels have been artificially manufactured with microfluidic networks of pores and throats, thus emulating the pore-scale geometries in porous media, for example, oil reservoir rocks. Micromodels manufactured in Si or glass have been used to visualize fluid flows in waterflooding experiments and two phase flow experiments, but their geometries have been limited to 2D pore network geometry. Realistic rock-based, 2.5D polymer micromodels made from the image of the Boise sandstone rock were developed for the measurements of 3D distributions of velocities and concentration of nanoparticles. Such 2.5D polymer micromodels enabled low cost manufacturing with replication-based process. However, studies of nano-particle mobility for in-reservoir applications require more realistic micromodels in terms of not only their 3D pore network geometries but also their materials, which are essentially similar to ceramics.

In this work, we present fabrication and flow visualization for rock-based, 2.5D ceramic micromodels. The 2.5D micromodels are 3D pore and throat networks with one wall flat (for observations) and the others fully 3D. The green ceramic precursors were batched using alumina powders and polymer binder mixture using a torque rheometer. The batch was used to extrude 3 mm thick green ceramic
tapes in a custom-made, rectangular extruder, which yielded shiny and flat tapes. Micromolding of the green ceramic tapes was performed in a conventional hydraulic press using a nickel mold in 13 layers fabricated using images of oil reservoir rock (Boise sandstone). The polymer binder mixture in the molded micromodels was removed by solvent extraction and thermal debinding. Sintering was carried out to densify the ceramic micromodel followed by sealing with a glass slide. Scanning electron microscopy inspection confirmed the distinct formation of 13 layers in the sintered ceramic micromodel, thus resembling the 3D pore network geometries of the 3D rock. The optical profilometer scan data showed the shrinkage of the ceramic micromodel after sintering (17.6% in x, 17.5% in y, and 16.4% in z).

Flow behaviors in 3D were investigated in the sealed ceramic micromodel using a confocal microscope with fluorescent dye and nanoparticles. The micromodel filled with dye showed good flow connectivity from bottom to top and fluorescence signal intensity dependence on depth. Fluorescent nanoparticles were injected at a flow rate of 30 nL/min and imaged in 5 μm depth increments. The overall flow patterns confirmed the similar principle flow paths as in the 2.5D polymer micromodel. A region of interest (ROI) with a least pressure resistant flow path was selected in the micromodel to investigate 3D variations of particle concentration and particle velocity. Peak particle concentration close to the observation window and gradual decrease in particle concentration along the depth were observed in the ROI. The ROI showed the higher velocities in the right throat (depth of 10 μm) due to lower flow resistance, and velocity variations along the depth. The rock-based, 2.5D ceramic micromodels will open a new avenue for the realization of rock-like micromodels from pulverized rocks with relevant pore geometry and material properties.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-F / 616

SAP-enhanced mortars: A multi-phase and multi-species modeling approach

Malte Sauerwein¹ ; Holger Steeb²

¹ M.Sc.
² University of Stuttgart

Corresponding Author(s): malte.sauerwein@mechbau.uni-stuttgart.de

In mechanized tunneling, grouting mortars are necessary for the backfilling of the annular gap, which is the cavity between the surrounding soil and the lining segments. An adequate grouting mortar should ensure a force-fitting connection in order to minimize surface settlements above the tunnel lining. The specific application prescribes two contrary requirements towards the rheology of the mortar mixture. On the one hand, a sufficient workability (low viscosity) is necessary for pumping the complex fluid through pipes into the gap, while this requirement can be fulfilled by starting with a high water content in the mixture. On the other hand, a rapid evolution of the mortar’s stiffness has to be ensured as soon as possible, which is usually initiated by a consolidation process. However, in the case of nearly impermeable soils, the dewatering process of the mortar would be too slow. The innovative concept of adding super absorbent polymers (SAPs) as an additive to the mortar mixture accelerates the gelation process. SAPs have the ability to absorb large amounts of the aqueous pore liquid in the mixture depending on the specific polymer characteristics and the chemical composition of the pore liquid. The SAPs swell to a hydrogel, while its mechanical properties differentiate tremendous from both the dry polymers and the free liquid.

In this contribution, the multiphase material is modeled within a continuum mixture theory based on the Theory of Porous Media (TPM). On the macroscale, the material is described as an immiscible mixture of three-phases. The solid phase represents the porous skeleton, while the pore space is simultaneously filled with a pore liquid and a hydrogel. Exchange terms in the mass balance equations for the phases account for the phase transition process on the macroscale, while the driving force for mass exchange has been modeled in accordance to well-established results in polymer physics. Both the chemical composition of the liquid phase and the properties of the hydrogel determine the
absorption capacity and the dynamics of water migration. Since chemical processes are involved, the multi-phase framework has been extended to a multi-species one. To this end, the pore liquid as well as the hydrogel are miscible mixtures of species. A strict exploitation of the entropy inequality according to the concept of Lagrangian multipliers proposed by Liu-Müller leads to admissible, thermodynamically-consistent constitutive models. The modeling parameters in the proposed mass exchange formulations have been identified by carrying out experimental swelling tests. Moreover, the reversible water absorption and desorption underlines the functional characteristics of the material. Modifying the composition of the pore liquid, e. g. the concentration of solved ions, affects the swelling properties strongly, while modeling predictions are in accordance to experimental results. Finally, the phase transition process, i. e. the swelling and deswelling of the SAPs, is coupled with the rheology of the mixture on the macroscale. Therefore, the mechanical properties of the mixture and the internal mass exchange are linked by the evolution of the internal state variables in the model.

References:
\bibitem{Alexandersson2016}
M. Alexandersson, H. Askfelt and M. Ristinmaa.
Triphasic Model of Heat and Moisture Transport with Internal Mass Exchange in Paperboard.
\bibitem{112:381-408,2016.}
\bibitem{Ristinmaa2011}
M. Ristinmaa, N.S. Ottosen and B. Johannesson.
Mixture theory for a thermoelasto-plastic porous solid considering fluid flow and internal mass exchange.
\bibitem{Bennetthum2011}
L. S. Bennethum and J. H. Cushman.
Multicomponent, Multiphase Thermodynamics of Swelling Porous Media with Electroquasistatics: I. Macroscale Field Equations.
\bibitem{Bennetthum2020}
\bibitem{Sauerwein2017}
M. Sauerwein and H. Steeb.
A modified effective stress principle for chemical active multiphase materials with internal mass exchange.
\bibitem{Geomechanics}
\bibitem{under review}
Acceptance of Terms and Conditions:

Click here to agree

**Poster 3 / 999**

**SH-TE acoustoelectric waves in double-cylindrical porous formation**

Zhiwen Cui\(^1\); Jinxia Liu\(^1\); Xiaoyan Zhu\(^1\)

\(^1\) Jilin University

**Corresponding Author(s):** cuizw@jlu.edu.cn

Due to the existence of electric double layer in fluid-saturated porous media, Acoustoelectric effect will occurred when acoustic waves propagate through media. In the logging while drilling environment the drilling collar might be taken as a shear source. SH-TE acoustoelectric logging is a potential method to obtaining shear wave velocity directed in LWD environments. When the interface exist out of the borehole, is it possible to use SH-TE acoustoelectric logging to estimate the interface? In order to simply our question, we consider the double-cylindrical formation model. We introduced the potential functions of SH-TE seismoelectric waves in porous formation. The expression of acoustic and electric/magnetic fields are obtained based on Pride theory and potential
functions. With the boundary conditions at fluid/inner-porous cylinder and the boundary conditions at inner/outer porous formation, the coefficients of the potential will determined. With the field equations, we calculated the transient waveforms of the electric or magnetic fields at any point along the borehole, and obtain the displacement of acoustic on the wall by digital Fourier transform. It is shown that there are five wave packets in the waveform of electric field. Two packets which reach simultaneously at recorders are generated at inner interface and outer interface. When the outer formation is homogenous, only one EM and SH wave packets will appear. The last two Love modes appear when the outer interface exists. One can obtain the acoustic velocity of SH wave and estimate the position of outer interface. It is a potential new method to detect the interface out the borehole using SH-TE acoustoelectric waves.

References:


Click here to agree

Parallel 5-A / 693

Salinity Effects During Two-Phase Flow in Porous Media: Electrokinetic Control of Viscous Fingering

Mohammad Mirzadeh1 ; Martin Bazant1

1 MIT

Corresponding Author(s): mirzadeh@mit.edu

Pattern formation is ubiquitous in many physical or chemical processes and has been at the center of attention for the past couple of decades. In many instances, interfacial instabilities play a central role in creating these patterns and controlling their spatiotemporal evolution. Perhaps one of the most well-known examples is the striking figures generated when a high-viscosity fluid is displaced by a low-viscosity fluid. This "viscous fingering" phenomenon was originally described by Saffman and Taylor in the context of Hele-Shaw flows but is also observed in porous media flows, where it leads to residual trapping during secondary or tertiary oil recovery and reduces extraction efficiency.

In the classical theory, the onset of instability is only controlled by a single parameter, i.e. the viscosity ratio. However, coupling with other physiochemical processes could enhance or suppress viscous fingering. For instance, many rock formations contain chemically active surface groups that dissociate in the presence of water and lead to the formation of surface charge. These surface charges interact electro-statically with mobile ions in the solution and can affect the flow behavior through the so-called electrokinetic coupling.

Here, we use linear stability theory as well as nonlinear numerical simulations to study the role of electrokinetic coupling and salinity effects on the interface stability. Our results indicate that viscous fingering may be controlled, and even suppressed, by applying external electric fields. Furthermore, even in the absence of electric fields, strong electrokinetic coupling (present in nanopores where the electric double layers overlap) can reduce viscous fingering by enhancing the "effective viscosity" of the injected fluid through the electro-viscous effect.
Our findings can have implications for electrically enhanced oil recovery application, as well as low salinity water flooding, and might help with understanding other similar multi-field driven interfacial instabilities.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-H / 460

Salinity and saturation dependence of the streaming potential coupling coefficient of porous carbonate rocks

Author(s): aurelien cherubini
Co-author(s): bruno garcia ; adrian cerepi ; andre revil

1 IFP Energies Nouvelles
2 ENSEGID
3 Université Savoie Mont-Blanc

Corresponding Author(s): aurelien.cherubini@ifpen.fr

The seismoelectric and self-potential methods are showing promises to characterize both the vadose zone of the Earth, hydrocarbon reservoirs and CO2 sequestration. That said, the dependence of a key parameter, the streaming potential coupling coefficient, with the saturation remains highly debated. We explore here the relationship between the streaming potential coupling coefficient, the water-gas saturation and the salinity in saturated and partially saturated carbonate rocks characterized by distinct textures. All the samples are saturated with NaCl brines, from 2.10-3 Mol L-1 to 2 Mol L-1. The magnitude of the coupling coefficient increases when the brine salinity decreases. Moreover, the streaming potential coupling coefficient seems independent of the nature of the rock in the range 2 – 600 mD. The core samples are characterized in terms of their porosity and intrinsic formation factor. A new core flooding system is used to measure simultaneously both the relative permeability, the resistivity index and the streaming potential coupling coefficient in steady-state two-phase flow conditions as a function of the saturation with CO2 or N2. The results are compared with a recently developed theoretical model, which can accommodate either the Brooks and Corey model. This model is predicting a set of relationships between the streaming potential coupling coefficient, the relative permeability and the second Archie’s exponent. We found a good agreement between the model based on the Brooks and Corey approach and experimental data.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-B / 632

Salinity-dependent transport of viruses in porous media

Dong Zhang ; Valentina Prigiojbe

1 Stevens Institute of Technology

Corresponding Author(s): dzhang18@stevens.edu
Urbanization in coastal areas can be a significant source of pathogenic microorganisms, such as viruses and fecal indicator bacteria. Recently, coastal water contamination is becoming an important issue due to global warming. Viruses can migrate long distances through porous media, such as beaches and coarse sediments, because of their biological characteristics, i.e., their size and motility. The attachment process of viruses onto soil grains can retard the virus transport, significantly. But, it can be reduced by the large salinity of the coastal water.

Here, a study that explores the effect of salinity on the instability of the virus front during transport in saturated porous media is presented. One dimensional (1D) transport model was developed following Cao et al. (2010) [2]. The model consists of two mass conservation equations of the virus and the salt concentration coupled through the constitutive equations of attachment/detachment mechanism. We observed that in the presence of hydrodynamic dispersion an instability develops at the virus front due to the formation of a mixing zone where the attachment is negligible. This instability develops in a pulse that travels at the speed of the average flow velocity. The magnitude of the pulse increases with the decreasing flow velocity.

References:

Click here to agree

Parallel 6-E / 891

Segmentation and Flow Characterization of Block Copolymer Ultrafiltration Membranes

M. Sadegh Riasi¹ ; Yuk Mun Li² ; Qi Zhang² ; Ulrich Wiesner² ; Lilit Yeghiazarian¹

¹ University of Cincinnati
² Cornell University

Corresponding Author(s): ms.riasi@gmail.com

Ultrafiltration membranes have a wide range of applications from drug delivery to water purification and virus filtration (Dorin et al. 2014; Li et al. 2017). A class of ultrafiltration membranes that has received much attention is the past decade is block copolymer membranes synthesized by self-assembly and non-solvent induced phase separation (SNIPS). These polymer membranes often exhibit an asymmetric, hierarchical structure comprising a thin (50-150 nm) separation layer with ordered nano-scale pores, and a support layer with a nanoporous solid matrix and disordered micro-scale pores.

Although optimizing flow is critical to the performance of such ultrafiltration membranes, not much success has been reported on their numerical flow characterization. The main challenges have been reported as i) hierarchical pore structure delineation (Sundaramoorthi et al. 2016) and ii) lack of an image-based micro-scale modeling approach that is computationally efficient and that can capture such wide pore size distribution (Shi et al. 2015).

In this study, we address the challenge of hierarchical pore structure delineation of an ISV triblock terpolymer membrane by combining a ~100 nm resolution 3D image of the membrane with high-resolution (2-4 nm) 2D SEM images. The 3D image is segmented using an automatic segmentation method (continuous max-flow algorithm) to delineate the micro-scale pores of the support layer. To capture the sub-resolution nanopores in the separation layer and in the solid matrix of the support layer, equivalent stochastic pore network models (PNM) of nanoporous structures are extracted from the high-resolution 2D SEM images.

To simulate single-phase flow, the pore topology method (PTM) is used. PTM is a fast micro-scale modeling approach that uses the medial surface of the 3D void space as the solution domain for flow simulation [Riasi et al. 2016]. After extracting the medial surface of the micropores, a local hydraulic conductivity and a solid matrix wall permeability coefficient is assigned to each voxel on the medial surface. The separation layer is then represented as a voxelized lattice structure assembled on top of the medial surface. The hydraulic conductivity of separation layer voxels and the wall permeability of solid matrix of support layer is acquired from the PNM analysis. Collectively, this provides the
solution domain, which is then used for single-phase flow simulation. Absolute permeability of the membrane is computed and compared with the experimental measurements.

References:


Acknowledgment of Terms and Conditions:

Click here to agree

Parallel 1-B / 391

Seismic monitoring of biopolymer accumulation and permeability reduction in sands

Dong-Hwa Noh\(^1\); Tae-Hyuk Kwon\(^1\)

\(^1\) Korea Advanced Institute of Science and Technology (KAIST)

Corresponding Author(s): dhnoh@kaist.ac.kr

Bacterial colonization and the spread of biopolymer, gel-like material, on porous media are known to decrease permeability by several order of magnitude and to cause biofouling thereby altering the hydraulic flow systems of porous media. Attention to microbial biofouling has been increasing owing to the increasing demand of microbial soil treatment and soil improvement. Successful microbial biofouling treatments require geophysical monitoring techniques to provide appropriate spatial and temporal information on bacterial growth and activities in the subsurface; such monitoring datasets can be used to evaluate the status of plugged sections and optimize re-treatment if the plug degrades. Therefore, this study investigated the feasibility of using P- and S-wave velocity and attenuation for monitoring the accumulation of bacterial biopolymers and the permeability variations during biofouling. In sand-packs, Leconostoc mesenteroides was cultured and stimulated to produce insoluble biopolymer and generate biofouling. During such bacterial biofouling, permeability and high-frequency P- and S-wave responses were monitored. P-wave velocity was consistent and S-wave velocity was increased with biopolymer accumulation. Both P- and S-wave attenuation, evaluated by using spectral ratio method, were increased with increasing biopolymer saturation. Increases in seismic attenuation are closely linked to the biopolymer saturation and permeability reduction. Herein, we also presented a theoretical model to correlate biopolymer saturation, permeability, and seismic attenuation by modifying three-phase Biot model and Pride-Berryman double-porosity model.

References:


Click here to agree

Parallel 1-C / 820

Self-healing cementitious blends with pozzolanic materials for subterranean applications

Tatiana Pyatina¹ ; Toshifumi Sugama¹

¹ Brookhaven National Laboratory

Corresponding Author(s): tpyatina@bnl.gov

Cement failure in subterranean wells may compromise zonal isolation, cause corrosion of steel casing and, in the worst case scenarios result in a catastrophic event of well collapse. Portland cement and its blends are used for cementing the majority of subterranean wells. Although they proved to provide a robust solution in many cases, they are not durable in aggressive environments with high total dissolved solids, acidic gases and fluids and large thermal and mechanical stresses. Although strong, cements in general are brittle and, as a result, may fractures or break under various stresses. Because of the difficulties in locating and accessing damaged areas in subterranean wells self-healing cements are of particular interest. Cementitious blends with pozzolanic materials may form resilient cements with self-reinforcing properties at longer curing times. This work revisits and updates applications of cementitious blends that include pozzolanic materials for carbonate-rich, strongly acidic high-temperature wells with large thermal and mechanical stresses. Data on strength recoveries and cracks sealing or bond re-formation for samples subjected to a repeated compressive damage followed by 5d 300oC healing periods in water, alkaline carbonate and geothermal brine are presented. Blend cements formation mechanisms, mechanical properties, resistance to mild and strong acids and cement/carbon steel bond characteristics and corrosion protection are discussed. Properties of the class G oil well Portland cement modified with silica for high-temperature applications are presented as a benchmark. Possible healing mechanisms based on XRD, Raman analyses and SEM coupled with EDX data are proposed. The evaluated pozzolanic materials include fly ash F, ground granulated blast furnace slag, natural zeolites, and micro glass fibers type E.

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 2-A / 509

Semi-Analytical Particle Tracking Scheme For Advective/Diffusive Transport in Porous Media

Daniel Meyer

1 Institute of Fluid Dynamics, ETH Zurich

Corresponding Author(s): meyerda@ethz.ch

Semi-Analytical Particle Tracking Scheme For Advective/Diffusive Transport in Porous Media

The particle tracking scheme of David W. Pollock [Ground Water 26(6), 1988] provides a computationally efficient and mass-conservative method for Lagrangian transport in the absence of diffusion. In this work, a generalization of Pollock’s scheme that allows for the inclusion of diffusion is presented. The new scheme is based on a semi-analytical representation of the advective/diffusive motion. The scheme does not require stepping at sub-grid-cell time or length-scales and thus is computationally efficient. It is formulated in such a way that it becomes exact for Pe going to zero and infinity, and provides an accurate numerical approximation in the intermediate Pe number range. Application examples dealing with Darcy flow in heterogeneous porous media and Stokes flow in resolved pore-space geometries document the capabilities of our new scheme.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 206

Semi-analytically derived flow-rate/pressure drop relationships for the flow of yield stress fluids through rectilinear pipes of non-circular cross-sections.

Azita AHMADI-SENICHAULT 1 ; Abdelaziz OMARI 1 ; Terence Emery MACKAYA 2

1 Professor, University of Bordeaux-FRANCE
2 PhD Candidate, E2M-TREFLE, ENSAM-Talence, FRANCE

Corresponding Author(s): azita.ahmadi-senichault@u-bordeaux.fr

For the study of yield stress fluids flow in porous media, the complex pore-scale structure has been extensively idealized as bundles of capillaries. A bundle of rectilinear capillaries of circular cross-section has been used over the past decade for the development of a new method of pore-size distribution (PSD) characterization based on the injection of a yield stress fluid. The main idea of this method, considered as an alternative to the mercury injection porosimetry, is that since those fluids cannot flow below a certain stress threshold, by measuring the evolution of the flow rate versus the pressure drop across a rock sample, its PSD can be retrieved through some “inversion” procedure. The numerical inversion techniques allowing to derive the PSD from experimental data and the experimental feasibility of this innovative and non toxic technique have been presented in recent works (e.g. Rodriguez de Castro et al., 2014). In order to be more representative of real pore cross sections, the flow rate/pressure drop relationship has been further investigated using detailed numerical simulations in bundles of capillaries with square or triangular cross-sections (Malvaut et al., 2017).

In this study we propose a set of semi-empirical formulas that relate flow rate and pressure drop for yield stress fluids flowing in rectilinear capillaries of square, triangular, and rectangular cross-sections. This approach is based on two main notions: the Critical Bingham number beyond which a yield stress fluid cannot flow anymore in a pipe of a given cross section; and a Shape Factor, whose physical meaning is the deviation of the considered shape of cross section (square, triangular, rectangular), from the ideal circular one.
This approach was initially proposed by Saramito and Roquet (2001) for the case of Bingham fluids flowing in pipes of square cross section. By following the same reasoning, a generalization for the flow of Herschel-Bulkley fluids in pipes of square, rectangular and triangular cross sections is developed.

The results obtained using the semi-analytical formulas developed in this work are shown to be in very good agreement with those derived from detailed numerical simulations. They can therefore be used for modeling flow in bundles of capillaries in a much more efficient and rapid manner.

References:


Click here to agree

Parallel 4-A / 868

Sensitivity of bare non-vegetated soil moisture dynamic simulations to prescribed soil-atmosphere interface boundary condition forcings

Author(s): Andrew Trautz

Co-author(s): Tissa Illangasekare; Stacy Howington; Abdullah Cihan

1 Colorado School of Mines
2 US Army Corps. Engineer Research and Development Center
3 Lawrence Berkeley National Laboratory

Corresponding Author(s): tillanga@mines.edu

Soil moisture is closely linked to the near-surface heat and mass transfer that couples the land and atmospheric states. The accurate simulation of the spatiotemporal distribution of soil moisture is constrained by existing knowledge gaps with respect to the mechanisms and processes linking the atmospheric and soil states, their magnitude, and sensitivity to applied soil conditions. In this study, we explore the effects of variations in microclimate conditions on state variable distributions and water balances for different bare soil conditions. A series of evaporative experiments were conducted at the Center for Experimental Study of Subsurface Environmental Processes (CESEP) wind tunnel- porous media test-facility to generate atmospheric and subsurface datasets that were in turn applied in the prescribed soil-atmosphere boundary conditions of a heat and mass transfer numerical model. Experimental results showed that for the length scale and edaphic conditions tested, variations in local soil-atmosphere coupling had a slight impact on the lateral distribution of soil moisture. This localized soil moisture variability could not be reproduced with numerical model. From a water balance perspective however, cumulative water loss could be adequately captured with little loss of fidelity. This demonstrates that heat and mass transfer models may be insensitive to the local microclimate driving bare-soil evaporation but are strongly influenced by local soil properties (i.e., heterogeneity). Together, these findings suggest that greater focus should be given to characterizing subsurface conditions and subsurface constitutive models and heat and mass transfer theory than localized near-surface atmosphere conditions.

References:

Acceptance of Terms and Conditions:

Click here to agree
Parallel 9-A / 508

Sensitivity studies of different scenarios of polymer injection applied to Ainsa Quarry1 outcrop

André Fournó¹ ; Jeanneth Zarate Rada¹ ; Noalwenn Dubos-Sallee¹ ; Veronique Gervais¹ ; Olivier Lerat² ; Patrick Rasolofosoana¹

¹ IFPEN
² ENSPM

Corresponding Author(s): andre.fourno@ifp.fr

The presented work deals with polymer injection in an oil reservoir of which the geological organization is obtained thanks to an outcrop located close to the Ainsa town in southern Pyrenees, Spain. In this study the permeability distributions are not fixed. We address the following question: what is the impact of permeability distribution on the oil recovery considering a polymer slug injection. This question makes sense because the outcrop may be an analogue of different types of reservoirs. Indeed the outcrop helps to characterize the facies distribution but has a different geological story compared to a subsurface reservoir. Three different reservoirs are thus considered to be associated to three permeability distributions, respectively corresponding to a non-altered reservoir, a fractured reservoir and an unconsolidated reservoir. The second permeability model results from an upscaling step in order to take into account the presence of fractures. The large permeability values of the third permeability model are due to unconsolidated facies. Models are respectively called "permeable" , "fractured" and "unconsolidated".

A water injection is modeled for 4 years with a pressure constraint of 500 bar. For each simulation, after a year of water flood, a polymer injection is carried out for two years. Finally, a water post-flush is injected until the end of the simulation. Polymer performance is tested against a water flood simulation whose final cumulated oil production equals to 0.2 hm3.

- Permeable model
  By injecting 0.21 hm3 of water, 0.21 hm3 of oil is produced. Due to weak facies permeabilities pressure reaches quickly the imposed limit. As a consequence, the water injection rate decreases during the water flood and, even more strongly when polymer is added to the solution. Therefore polymer injection does not help to better produce oil in the permeable model.

- Fractured model
  0.28 hm3 of oil and 0.2 hm3 of water are produced by injecting 0.65 hm3 of water. The produced water volume ratio (with and without polymer) is reduced by ~70%. Polymer injection is quite appropriate in this case since enhanced oil recovery reaches 40%.

- Unconsolidated sandstone
  0.23 hm3 of oil is produced after injecting 0.87 hm3 of water. The high permeability allowed the injection of larger volumes of water and polymer solution. However, the oil recovery volume is decreased in comparison to the fractured case. An earlier water breakthrough and a higher produced water volume contribute to this bad performance.

As a conclusion, the polymer impact critically depends on the permeability distributions. If the reservoir permeability is too weak it will be difficult to inject polymer without damaging the reservoir or the injection wells. If the reservoir is too permeable, an earlier water breakthrough is observed which has a negative impact on oil production.

References:

Acceptance of Terms and Conditions:

Click here to agree
Sequential data assimilation with multiple nonlinear models and applications to subsurface flow

Wanb Peng¹ ; Lun Yang¹ ; Akil Narayan²

¹ Beihang University
² University of Utah

Corresponding Author(s): wang.peng@buaa.edu.cn

Complex systems are often described with competing models. Such divergence of interpretation on the system may stem from model fidelity, mathematical simplicity, and more generally, our limited knowledge of the underlying processes. Meanwhile, available but limited observations of system state could further complicate one’s prediction choices. Over the years, data assimilation techniques, such as the Kalman filter, have become essential tools for improved system estimation by incorporating both models forecast and measurement; but its potential to mitigate the impacts of aforementioned model-form uncertainty has yet to be developed. Based on an earlier study of Multi-model Kalman filter, we propose a novel framework to assimilate multiple models with observation data for nonlinear systems, using extended Kalman filter, ensemble Kalman filter and particle filter, respectively. Through numerical examples of subsurface flow, we demonstrate that the new assimilation framework provides an effective and improved forecast of system behavior.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-D / 586

Shape analysis for grains and pores on 3d digital images

Fabian Biebl¹ ; Tom Cvjetkovic¹ ; Erik Glatt¹ ; Andreas Wiegmann¹

¹ Math2Market

Corresponding Author(s): fabian.biebl@math2market.de

With our Software GeoDict® we are able to segment 3d scans, e.g. CT or FIB-SEM scans. This segmented data can then be analyzed using GeoDict’s new modules GrainFind and PoreFind. In this talk, we introduce GeoDict and present the features of these two modules.

For each individual pore, PoreFind extracts an equivalent ellipsoid from the segmented data. From the equivalent ellipsoids, we get the statistics of pore positions, pore orientations, and size distributions. Another property is the sphericity of the pore. These statistics can be used to provide parameters for engineering models as needed in [2], for example, to predict properties of rocks.

For each individual grain, GrainFind extracts an equivalent ellipsoid from the segmented data. From the equivalent ellipsoids, we get the statistics of grain positions, grain orientations, and size distributions. Another property is the sphericity of the grain. From these statistics, one can create a virtual twin of the scan, i.e. one has a computer model that allows the creation of voxelized 3d grain models with the same statistics. Furthermore, with GeoDict, this virtual twin can be used as a starting point such that it may better fit to those physical properties you want to optimize. One such property, for example, is the tortuosity of electrode materials as considered in [3].

References:

Parallel 9-B / 49

Short timescale wetting and liquid penetration on porous media, an experimental approach

Michael Richter\textsuperscript{1}\textsuperscript{none}; Oliver Hunstein\textsuperscript{1}\textsuperscript{none}; Ulrich Hirn\textsuperscript{1}; Sarah Krainer\textsuperscript{2}

\textsuperscript{1} Graz University of Technology
\textsuperscript{2} Technical University of Graz

Corresponding Author(s): sarah.krainer@tugraz.at

Paper curl due to wetting and drying is known to be determined by the degree of fiber swelling, the paper structure and material inner tensions from the paper production process which are released due to wetting. Apart from these well documented processes we have found that the development of paper curl is governed by different mechanisms depending on the observed time domain.

Our investigation shows that different curl mechanisms are taking place during initial wetting, immediately after paper drying and during the first 48 hours after printing. Accordingly we are defining three different types of curl: initial wetting curl, short term print curl and long term print curl. Initial wetting curl is defined to take place in the first few seconds after contact with the printing ink. Short term print curl is defined as the paper curl occurring directly after printing and drying of the printed paper. Long term printing curl is the paper curl occurring 24 hours after printing and drying of the paper.

An analysis of the reasons for the development of paper curl in the different time scales revealed that initial wetting curl seems to be related to the fiber swelling, short term printing curl is related to the structure of the paper and long term curl is triggered by re-conditioning the paper after printing.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-B / 48

Short timescale wetting and penetration on paper

Author(s): Sarah Krainer\textsuperscript{1}

Co-author(s): Ulrich Hirn \textsuperscript{1}

\textsuperscript{1} Technical University of Graz

Corresponding Author(s): sarah.krainer@tugraz.at

In this study penetration and spreading of printing ink on paper in High Speed Inkjet (HSI) printing is investigated. Printing ink penetration is reducing color density and spreading of the ink on the surface is crucial for development of print density. Three measurement techniques are evaluated: Ultrasonic liquid penetration measurement (ULP), contact angle measurement (CA) and scanning absorptometry (SA). With each of these techniques liquid penetration as well as surface wetting can
be measured. For our studies we are using model liquids with defined surface tension, viscosity and polarity in terms of Hansen solubility parameters. A quantitative comparison of these three measurement techniques is carried out. Two parameters indicating a combined parameter for liquid penetration and wetting are introduced. The slope of the contact angle over time and a contact angle calculated from SA by rescaling according to the Lucas Washburn equation. These two parameters are correlated, supporting the idea that they are indeed capturing a combination of liquid penetration and wetting.

Furthermore, we want to investigate parameters, which are responsible for the absorption behaviour and how strongly they affect it. Starting with looking at the influence of viscosity and surface tension. For the investigation of these properties in the HSI printing process an industrial print head is used. We introduce the Ohnesorge – Number and Reynolds-Number to take advantage of the whole operation window of the print head and develop liquids, which are at the very limit of (good) jet-ability, in terms of surface tension and viscosity. Full.prints are analysed with a print-through method and a single droplet evaluation is done with an image analysis program. To close the circle these liquids are also measured with the ULP, SA and Contact angle measurement (CA also using picoliter-droplets) to see how the print results correlate with the measurement results.

References:

Acceptance of Terms and Conditions:

Click here to agree

---

Poster 3 / 853

Similarity of water movement in porous media under the conditions of microgravity and hydrophobicity

Kosuke Noborio¹ ; Naoto Sato²

¹ Meiji University
² Meiji University

Corresponding Author(s): nobori@meiji.ac.jp

A water infiltration rate into soil or porous media is reported to be slower in microgravity than on the earth with 1G (Jones and Or, 1999) as well as for hydrophobic soils (DeBano, 1971). Water characteristic curves under the microgravity condition (Heinse et al., 2007) and for hydrophobic soils (Bauters et al., 2000) very much look alike little changes in matric potential with various water contents. For hydrophobic soils (Bauters et al., 2000), the water contact angle becomes larger as well as under microgravity for larger droplets (Brutin et al., 2009). We thought that the contact angle might play the key role for water infiltration under microgravity. We will discuss more on this matter from the view point of similarity between microgravity and hydrophobicity at the minisymposium.

References:


Click here to agree
Simulation of Isothermal Drying of Porous Media using Lattice Boltzmann Method

Author(s): Githin Tom Zachariah
Co-author(s): Vikranth Kumar Surasani

1 Student
2 Professor

Corresponding Author(s):

Drying is a highly energy intensive unit operation in the process industry. Its high complexity due to the large number of interacting phenomena makes it very difficult to model. Thus far, modelling of drying was done using either continuum methods or pore network models, both of which have some limitations. In this work, the Lattice Boltzmann Method (LBM) is used to simulate the drying in porous media. The LBM is ideal for such simulations as it can incorporate complex effects in a simple and natural way. Four different types of porous media were used, differing in both node and throat geometries.

Due to the complex geometries present in porous media, capillary instabilities are often observed which leads to sudden jumps in drying rate. In this work, the effects of such instabilities on the liquid distribution is studied and an approximate range of such effects is identified. Further, we compare the drying of different types of porous media to identify the dependency of capillary instabilities on the pore structure. It was observed that the types of liquid interface motion could be classified into two types- type A, which constituted of slow invasion of pores by diffusion and type B, which involved fast invasion of voids due to capillary instabilities. It was observed that some types of porous media exhibited an abundance of type A invasion, while others showed a combination of type A and type B. Lastly, it was observed that the drying rate of nodes depend heavily on it structure. Nodes with sharp edges take considerably longer to invade due to liquid holdup at the edges. This work emphasizes the advantages of using the LBM for modelling drying of porous media.

References:


Acceptance of Terms and Conditions:
Click here to agree

Simulation of Metabolic Processes in Plant Cells

Tobias Elbingler; Peter Knabner

1 Friedrich-Alexander-Universität Erlangen-Nürnberg

Corresponding Author(s): elbingler@math.fau.de

The interior of living cells can be considered as a porous medium consisting of three compartments: cytosol, chloroplasts and mitochondria. Diffusion and reactions take place inside the cytosol, inside the chloroplasts and on the surfaces of the mitochondria. Furthermore, biochemical species can be exchanged between the compartments. Consequently we need to solve a system of fully dimensional partial differential equations coupled with partial differential equations on lower dimensional
manifolds. The nonlinear coupling terms result from reversible enzyme kinetics. We present an efficient algorithm for solving this system on parallel machines and investigate the role of enzyme localization on the mitochondria surfaces.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 4 / 517

Simulation of elasto-plastic phenomena in heterogeneous soils using the Virtual Element Method

Andrea Borio¹ ; Stefano Berrone² ; Stefano Scialò¹ ; Alessandro D'Auria¹ ; Fabio Vicini¹

¹ Politecnico di Torino
² Politecnico di Torino, Italy

Corresponding Author(s): andrea.borio@polito.it

The three-dimensional version of the Virtual Element Method is a field under great development, both from the theoretical point of view [1] and the implementation aspects [2]. The simulation of the flow inside a poro-fractured medium has been recently tackled using the Virtual Element Method in the context of Discrete Fracture Networks [3–6]. Here we consider the threatment of non linear elasto-plastic phenomena with such method, with particular focus on phenomena occurring within heterogeneous poro-fractured soils with faults, generated by petrol related operations such has the introduction of wells that modify the pressure distribution in the subsoil. Virtual Elements are used in order to simplify the meshing process in the presence of complex geometries, allowing the use of generally shaped polyhedra.

References:


Click here to agree

Invited 3 (Room C) - Géraldine Pichot / 495

Simulation of flow properties in geological-based Discrete Fracture Networks
Fractures are crucial in the physics of geological media and have specific characteristics different from the surrounding rock matrix. Addressing their bulk hydraulic behavior is challenged by the multiscale fracture heterogeneities without any obvious homogenization scale and persistent high-flow channeling. Predictive flow simulations based on geological characterization are essential but face involved geometrical and computational issues. We propose here new combinations of advanced mesh generation methods and robust numerical schemes together with vectorization to solve the flow problem at a moderate cost.

Our approach relies on advanced methods for geometric modeling and mesh generation that are implemented in the BLSURF_FRAC software. It first builds an analytic model of the intersecting fractures. Then, using BLSURF [1], it discretizes the intersections and fracture contours and generates corresponding surface meshes. Automatic corrections are added to ensure valid meshes for any fracture structures. Mesh generation is performed either by BAMG [2] or BL2D [3]. Meshes can be adaptively refined to optimize flow computations.

On top of it, the GeoFlacflow software provides hydraulic simulation capacities with an optimized implementation of the mixed hybrid finite element method with vectorization [4] to reduce computational times. It handles either matching or non-matching meshes at the intersections between fractures [5], sink/source terms and high contrasts of transmissivities between fractures.

We benchmark our proposed methods by computing flow properties of geological-based Discrete Fracture Networks [6, 7] including correlations between fractures (UFMs) [8]. They are large-scale DFNs where the fracture size distribution matches the observations and where fractures are organized so that large fractures inhibit the growth of smaller ones, creating T-termination configurations. We also show possible optimization capacities offered by optimal combinations of mesh generation methods (BAMG or BL2D) and the mixed hybrid finite element method.

Bibliography


References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 11-C / 72

Simulation of injectivity decline in fractured near-well regions
Xavier Raynaud

1 SINTEF

Corresponding Author(s): xavier.raynaud@sintef.no

Accumulation of large particles on well faces decreases the injectivity. This issue is particularly acute in the case of produced water reinjection (PWRI) and polymer flooding. To maintain operational rates, the injection pressure is increased, which causes fracturing or reopening of existing fractures. Then, the injectivity may be recovered or even increased, but only temporarily, as filter cakes start building up on the freshly opened fracture walls. In this talk, we will show simulation results of injectivity decline. We will present the models and the simulation methods we have chosen for the main relevant processes: Transport in discrete fracture networks for the large particles, external filter cake build-up on the fracture faces, poroelasticity to determine the fracture apertures.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-A / 946

Simulation of particle straining in porous media using a coupled pore-network and CFD-DEM model

Author(s): Hongtao Yang

Co-author(s): Zhuang Sun 1; Matthew Balhoff 2

1 The University of Texas at Austin
2 University of Texas at Austin

Corresponding Author(s): hongtao.yang@utexas.edu

Geometrical straining of particles in porous media is of critical importance in a broad range of natural and industrial settings, such as the contaminants transport in aquifers and the permeability decline due to pore plugging in oil reservoirs. Despite its importance, relatively few studies have been performed on particle straining under fluid-driven flows in porous media. Pore-network modeling is attractive for predicting particle straining. However, network models often lack predictive capability due to simplification of pore-geometry and require adjustable parameters. This is especially true for particle straining. Direct numerical simulation using computational fluid dynamics (CFD) to model the fluid phase, coupled with the discrete element method (DEM) to model the particle transport is a more rigorous approach but computationally expensive. The CFD-DEM simulations are limited to systems with particle number less than 105.

Our current research has coupled a pore network model with a CFD-DEM model in a computationally-efficient framework. Particle jamming is a matter of probability. We perform CFD-DEM simulations on particle filtration by a single layer of grains and formulate the jamming probability as a function of particle/pore size ratio, particle concentration, pore throat geometry etc. The upscaled results are then implemented into the pore-network model. During a time step, the jamming probability of each pore throat is calculated based on the local particle concentration, flow rate etc. The hydraulic conductivities of pore throats are updated dynamically. The numerical results are compared to direct CFD-DEM and experiment results and good agreement is achieved.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 8-F / 118

Simulation of two-phase flow by diffuse interface methods

Beatrice Riviere, Florian Frank, Chen Liu, Faruk Alpak

Corresponding Author(s):

Diffuse interface methods are popular methods for modeling two-phase flow at the pore scale. These methods are based on the minimization of Helmholtz free energy of the fluid system and approximate the interface between the phases by a transition region of finite thickness. The mathematical model is a coupled system of time-dependent Cahn-Hilliard and Navier-Stokes equations. Contact angle is imposed on each rock-fluid interface via a boundary condition. We discretize the differential operators in space by the interior penalty discontinuous Galerkin methods. For the Cahn-Hilliard equations, we use a convex-concave splitting of the chemical energy density. For the Navier-Stokes equations, we employ a pressure-correction projection algorithm. We validate the method on a series of benchmark problems.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 2 / 369

Single-scale heterogeneous pore network modelling with micro-porosity upscaling.

Nijat Hakimov, Arsalan Zolfaghari, Amirmasoud Kalantari-Dahaghi, Shahin Negahban, Arash Aghaei

1 University of Kansas
2 TORP/University of Kansas
3 Thermo Fisher Scientific

Corresponding Author(s): hakimov@ku.edu

One of the longstanding challenges of the oil and gas industry is the problem of scale and hence, the term “upscaling” is used frequently in literature. In this work, we investigate the ways to represent connected regions with substantially different pore sizes. For this purpose, pore-scale simulations are combined with conventional continuum scale models. Our primary objective is to run sensitivity analysis considering topology changes for the pore space above and below a given resolution. Inspired by conventional upscaling practices, we assign upscaled flow properties to a group of pores and throats that are smaller than a given resolution. We show if the back calculated upscaled properties are solely a function of the pore space topologies at smaller scale. To make our study more general, we also investigate different pore-to-pore connections at larger scales. First, we start by considering the simplest case where two macro-pores connected through cuboidal regular lattice network of micro-pores that represents microporous region. Calculating upscaled properties of the cuboidal lattice, we compare results from both conventional pore-scale and hybrid upscaled models. Consequently, we vary pore space connectivities within the cuboidal lattice as well as the connectivity with macro-pores to study a wide range of possible scenarios for these two different scales of pores. The results could provide insight to our understanding of multiphase flow in rocks with different scales of importance and upscaling large pore networks to speed up pore-scale simulations.

References:

Acceptance of Terms and Conditions:

Click here to agree
**Poster 2 / 642**

**Slow Redistribution of Capillary Trapped Gas in Heterogeneous Porous Medium**

Michal Snehota¹ ; Jan Sacha² ; Tomas Princ³ ; Jan Hovind⁴

¹ Czech Technical University in Prague, Civil Engineering  
² Czech Technical University in Prague  
³ Czech Technical University in Prague  
⁴ Paul Scherrer Institut, Laboratory for Neutron Scattering and Imaging

**Corresponding Author(s):** tomas.princ@fsv.cvut.cz

Infiltration is the key hydrological process that affects a formation of runoff, floods generation, water erosion, and leaching of contaminants through soil. These processes are often most intensive in nearly saturated soils. An example of frequently highly saturated and intensively leached soils are the filter layers of the storm water infiltration swales, bioretention cells, and rain gardens. It was shown that soils rarely reach full water saturation, thus clusters of residual air reside in pores [1]. The consequences of partial water saturation are the increased gas storage and reduced hydraulic conductivity [2]. The extent of the impact of trapped air on soil water processes depends on the amount of entrapped air, and even more, on its spatial distribution [3] within the pore space. Recent experiments showed that neutron tomography has sufficient sensitivity to quantitatively detect small changes of water content, and thus the changes of trapped air content in dual-porosity material [4]. The aim of this study was to assess quantitatively the air trapping and subsequent slow redistribution in the dual-permeability material during water flow as well as during situation at which water in the nearly saturated soil does not flow.

Redistribution of trapped gas was quantitatively studied by three-dimensional (3D) neutron imaging in series of experiments conducted on a sample composed of fine porous ceramic and coarse sand. The redistribution of water was studied under both no-flow and steady state flow conditions. A series of ponded infiltration experiments was conducted on a sample by delivering heavy water with a peristaltic pump to the top of the sample while maintaining a constant water level. The water was allowed to flow freely by gravity through the perforated disc at the bottom of the sample. Four continuous and three intermittent infiltration runs were conducted on the sample with different initial water contents. The neutron imaging was conducted at Neutron Radiography (NEUTRA) beam line of the Swiss Neutron Spallation Source (SINQ) at the Paul Scherrer Institute (PSI) in Villigen, Switzerland [5]. A total number of 69 tomography images were taken for this study. Images that represented the three-dimensional spatiotemporal distribution of air and water in the sample were calculated with use of images of fully saturated and dry sample [6]. Based on the robust experience of visualization of the flow within heterogeneous samples, it seems that due to the huge local (microscopic) pressure gradients between contrasting pore radii the portion of faster flowing water becomes attracted into small pores of high capillary pressure. The process depends on the initial distribution of entrapped air which has to be considered as random in dependence on the history and circumstances of wetting/drying. The rate of the redistribution was significantly higher in the case of steady state flow condition in comparison to no-flow conditions. Imaging also demonstrates that residual air accumulated preferentially on the interfaces between coarse sand and fine ceramics. The transfer from fine to large pores leads to the reduced hydraulic conductivity of the sample.

**References:**

Sodium chloride crystallization in confinement: The mechanism of cubic to hopper crystal growth transition

Hannelore Derluyn\textsuperscript{1}; Julie Desarnaud\textsuperscript{2}; Jan Carmelië\textsuperscript{3}; Daniel Bonn\textsuperscript{4}; Nounash Shahidzadeh\textsuperscript{2}

\textsuperscript{1} CNRS - Univ Pau & Pays Adour \\
\textsuperscript{2} University of Amsterdam - Institute of Physics \\
\textsuperscript{3} ETHZ \\
\textsuperscript{4} University of Amsterdam

Corresponding Author(s): hannelore.derluyn@univ-pau.fr

Sodium chloride crystallization is a key factor in many industrial and geological processes such as for deicing salts, in oil well drilling and CO2 sequestration, in the erosion of rocks, monuments and for the sodification of soils. Generally, salt crystallization in confined space, as encountered in porous media, can significantly change the porosity and permeability, and as such restrict flow and mass transfer; in addition it can even deform the solid matrix due to the build-up of a crystallization pressure. Therefore, the ability to influence the rate of the crystal growth and the resulting morphology can have a significant impact on various applications.

We report on the transition mechanism from cubic to hopper growth of sodium chloride and the supersaturation at which the transition is observed. For this we have investigated experimentally at the microscale the kinetics of crystal growth at different degrees of supersaturation $S$ in confinement, up to its metastability limit which happens at $S = 1.6\pm0.2$ times the saturation concentration\textsuperscript{3}. The growth rates at the onset of precipitation are quantified together with the corresponding supersaturation. Our results show that the growth rate of the cubic crystal increases linearly with increasing supersaturation up to $S = 1.4$, which corresponds to the lower limit of the metastability. Surprisingly, above this supersaturation, the cubic growth rate levels off to a maximal rate of $6\pm2 \mu m/s$. By combining the global growth coefficient derived from our measurements with those in the literature at different temperatures, we corroborate the activation energy for the growth of sodium chloride.

For supersaturations above 1.4, as the cubic crystal cannot grow any faster, the hopper growth is initiated in order to consume the supersaturation rapidly; the hopper growth shows up as a chain-like structure of small cubic crystals. We show that the speed of the total hopper growth is much faster than the determined maximal speed of the growth of each cubic unit. Our experimental results of growth speed as a function of supersaturation above 1.4 can be fitted with a power law with an exponent of 3, underlining a two dimensional nucleation growth mechanism \textsuperscript{2}. The hopper morphology disappears at a later stage of growth if there is enough salt solution to supply the crystal with ions to continue the cubic growth at very low supersaturation.

Although hopper growth has been reported for different salts, this study is the first one in which the mechanism of such growth morphology is clearly identified and experimentally measured. Understanding the crystallization pathways allows to better control crystal design or to elucidate on pore-space changes as occurring during e.g. salt weathering of rocks and building materials or CO2 sequestration, and to enrich geochemical models.

References:


Acceptance of Terms and Conditions:

Click here to agree.
Poster 2 / 602

Soft fillings in nanoporous solids: Electro-polymerization and mechanical characterization of polypyrrole in nanoporous silicon

Manuel Brinker1 ; Stella Gries1 ; Pirmin Lakner2 ; Tommy Hofmann3 ; Thomas Kellerhorns ; Patrick Huber1

1 Hamburg University of Technology
2 Deutsches Elektronen-Synchrotron (DESY)
3 Helmholtz Zentrum Berlin

Corresponding Author(s):

We investigate the properties of the electrically conductive polymer Polypyrrole (PPy) in tubular pores of monolithic micro (pore diameter D < 2 nm), meso- (2 nm < D <20 nm) and macroporous (D > 50 nm) silicon. We successfully demonstrate a homogeneous filling via electro-polymerisation for the extremely anisotropic confinement of 12 nm pore diameter and 180 µm pore length. The kinetics of this process are explored experimentally and related to phenomenological models for polymerization in confined geometries. First experiments on the enhancement of mechanical properties of the resulting soft-hard nanohybrids are also presented.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-B / 935

Soil bacteria: searching for more efficient bio-fertilizers

Sofia Montagna1 ; Verónica I. Marconii

1 FAMAF-UNC
2 FaMAF-UNC and IFEG-(UNC-CONICET)

Corresponding Author(s): vmarconi@famaf.unc.edu.ar

Life in porous media, as soil bacteria, are used since more than 40 years ago as bio-fertilizer contributing to the development of a sustainable agronomy. Even though they are extensively used due to their low cost, such biotechnology is still far from being efficient and many challenges are opened for basic research in porous media science.

Our microbiological system of study are the Bradyrhizobium diazoefficiens, bi-flagellar bacteria. One of the opened question regarding its efficiency is which is the aim of its bi-flagellum system developed by this specie and not developed in general in Bradyrhizobium. It may be an adaptive trade-off between energetic costs and ecological benefits among different species. We work interdisciplinary on bacteria diffusion in porous media, numerically and experimentally, imitating the complex and structured soil with artificial micro-fluidics devices. With a better visualization in transparent devices, easy to manipulate in a laboratory we aim to understand and control the transport properties of the system for further realistic applications. In this work we were able to report numerically their recent reported strategies to swim [Quelas et al, Sci.Rep. 2016]. Further we simulate their dynamics with those realistic parameters, under a broad spectrum of micro-confinement environments, contributing to micro-fabricate different geometries of porous media. All these studies contribute to understand their diffusion properties versus their flagellar systems (different motility) and versus the porous arrangement. These in vitro contributions hopefully will be useful for further development in a sustainable agronomy.

References:
Solute dispersion for stable density-driven flow in randomly heterogeneous porous media

Aronne Dell’Oca, Monica Riva, Jesus Carrera, Alberto Gudagnini

1 Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
2 Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
3 GHS UPC-CSIC, IDAEA, CSIC

Corresponding Author(s): monica.riva@polimi.it, alberto.gudagnini@polimi.it

We present a theoretical investigation on the processes underpinning the reduced longitudinal spreading documented in stable variable density flows, as opposed to constant density settings, within heterogeneous porous media. We do so by decomposing velocity and pressure in terms of stationary and dynamic components. The former corresponds to the solution of the constant density flow problem, while the latter accounts for the effects induced by density variability. We focus on a stable flow configuration and analyze the longitudinal spread of saltwater injected from the bottom of a column formed by a heterogeneous porous medium initially fully saturated by freshwater. We adopt a perturbation expansion approach and derive the equations satisfied by section-averaged concentrations and their ensemble mean values. These formulations are respectively characterized by a single realization and an ensemble dispersive flux, which we determine through appropriate closure equations. The latter are solved via semi-analytical and numerical approaches. Our formulations and associated results enable us to discriminate the relative impact on the density-driven solute displacement of (a) covariance of the permeability of the porous medium, (b) cross-covariance between permeability and concentration, which is in turn linked to the coupling of flow and transport problems, and (c) cross-covariance between the dynamic and stationary velocities.

Solute mixing during immiscible displacements in porous media

Author(s): Sayed Alireza Hosseinzadeh Hejazi

Co-author(s): Takeshi Kurotory, Saurabh Shah, Ronny Pini

1 Imperial College London

Corresponding Author(s): takeshi.kurotory13@imperial.ac.uk

Understanding the nature of solute transport in the subsurface is important for applications such as CO2 storage in deep saline aquifers and the extraction of oil and gas from deep sandstone or carbonate formations. However, limited knowledge exists in this area due to the extent of heterogeneity in geological formations and the additional complexity coming from presence of multiple fluid phases. Heterogeneity plays a key role in these natural environments; the latter is manifested through the spatial variability of petrophysical properties, which in turns creates preferential flow paths and
results in significant lateral spreading of the solute plume. The main focus of this study is to understand the effect of permeability heterogeneity on solute mixing and spreading in the presence of a second immiscible fluid phase. To this aim, single- and multi-phase pulse-tracer experiments were conducted on both unconsolidated systems (beadpack) and reservoir cores (Bentheimer Sandstone) using the N2/water system, and breakthrough curves were measured. X-Ray Computed tomography (CT) and Positron Emission Tomography (PET) were used to obtain 3D distribution of fluid phase saturations and to simultaneously image the dynamic displacement of a radiotracer within the sample, respectively. In addition to the conventional transmission-mode tracer test, the “echo” technique is applied to decouple spreading introduced by (relative) permeability heterogeneity and Fickian mixing. The postulate tested here is whether the trapped non-wetting phase introduces a similar spreading mechanism, as would be expected from varying grain sizes in a single-phase scenario, and if this additional advective distortion is reversible in “echo” mode pulse-tracer tests. This is of paramount importance for investigating the extent of mixing caused by heterogeneity in multiphase flow systems and to identify a correlation between dispersivity and fluid saturation in various reservoir cores.

In this study, we have validated the ability of the “echo” technique to describe heterogeneous systems with conventional advection dispersion equation (ADE) for both single- and multi-phase cases. This in turns provides a simple reliable approach to obtain intrinsic dispersivity of a heterogeneous porous system over a wide range of nonwetting saturation levels (~0.0 to 0.5). We observe (i) that dispersivity does depend on the saturation level of the non-wetting phase and (ii) that this dependency is stronger in the beadpack system as compared to Bentheimer Sandstone. We contend that this is due to an inherently different microscopic configuration of the trapped ganglia in the pore space of unconsolidated and consolidated systems, as supported through images acquired at higher resolution on an X-ray microCT scanner.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-A / 832

Sorption Stresses in Organic-Rich Rock Formations: Fundamental Processes and Reservoir Scale Implications

Igor Shovkun¹ ; D. Nicolas Espinoza¹

¹ The University of Texas at Austin

Corresponding Author(s): espinoza@austin.utexas.edu

Hydrocarbon sorption in unconventional formations accounts for a significant amount of gas in place depending on rock mineralogy and organic content. Traditionally, sorption amount experiments have been performed on powders or crushed porous solids that ignore changes in pore structure.

Dilatometry experiments, however, show that changes of volume during sorption can result in dramatic changes to porosity structure that alter the organic-rich nanoporous solid. The maximum linear swelling strains in natural nanoporous media such as coal and shale caused by sorption of light hydrocarbons and CO2 vary from 0.05% to 1% and differ with respect to the orientation to deposition bedding.

An organic-rich nanoporous solid exposed to a sorbate and constrained to do not deform, develops sorption stresses rather than sorption strains. The sorption stress was measured in coal with values as large as ~40 MPa at a CO2 bulk pressure of 5 MPa. Direct measurements of desorption stress have also been done in coal with CH4.

In this work we show a comprehensive review of sorption-induced strains and stresses in organic-rich rocks. We use these laboratory measurements in an up-scaled reservoir model that permits quantifying the effects of sorption-induced stresses on fracture permeability and on production rates. We compare cases of coal and shale natural gas reservoirs.

The results show that gas desorption-induced stresses have a significant effect on the evolution of stresses in the reservoir and therefore on the permeability of natural and induced fractures.
References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-E / 700

Sorption of Methane and Carbon Dioxide in Type II-A Kerogen Rough Slit Nanopores by Molecular Simulations

Stephane TESSON¹ ; Abbas HIROOZABADI²

¹ Reservoir Engineering Research Institute (RERI) & University of California Riverside (UCR)
² Reservoir Engineering Research Institute (RERI)

Corresponding Author(s): stesson@rerinst.org

Shale gas has redefined energy landscape. The United States (U.S.) natural gas production is expected to increase every year, and in 2035 the U.S. shale gas production may raise to 50% of the total gas production.

Shale rock consists of micropores and mesopores[2]. It is also composed of inorganic minerals (quartz, clays, calcites, and feldspars, etc.) and organic matter (kerogens and bitumens). The organic matter is mainly composed of kerogens and it is considered as the main gas trapping of methane[3] and shows high capacity for carbon dioxide adsorption trapping[4]. An understanding of shale kerogen adsorption characteristics, under the reservoir condition, is required to successfully exploit the shale formations.

Three different types of kerogen depending on its origin can be distinguished: i) type I from a lacustrine anoxic environment, ii) type II from marine shale and continental planktons, and iii) type III from plants in tertiary and quaternary coals. All these types can be classified according to the elemental ratio of Hydrogen/Carbon (H/C), Oxygen/Carbon (O/C), and Sulfur/Carbon (S/C). The physicochemical properties (structure, adsorption, retention, etc.) of the kerogen strongly depend on its origin and on the burial history of the reservoir where it came from[5].

Molecular simulations allow a detailed picture of the structure, thermodynamics and dynamics of the fluid at the interface. In this work the dry structures of type II immature kerogen with different types of dummy particles are simulated. Then, the kerogen media are used to study the sorption of methane and carbon dioxide in the kerogen matrix and at the kerogen rough slit nanopore surface. Our results are compared with the available experimental data.

References:


Click here to agree

Parallel 10-F / 110

Spatial correlation of contact angle and curvature in pore-space images
Ahmed AlRatout1; Martin J. Blunt1; Branko Bijeljic1

1 Imperial College London

Corresponding Author(s): b.bijeljic@imperial.ac.uk

We study the in situ measured distributions of contact angles and curvatures within mm-size X-ray tomography images of rock samples from a producing hydrocarbon carbonate reservoir imaged after waterflooding. We analyse their spatial correlation on a pore-by-pore basis using automated methods for measuring contact angles [2], a new method for measuring curvatures, and by performing pore network extraction using generalized network modeling [3]. The automated methods allow us to study image volumes of diameter approximately 1.92 mm and 1.2 mm long, obtaining hundreds of thousands of values from a dataset with 435 million voxels. We calculate the capillary pressure based on the mode curvature value, and associate this value with a nearby throat, or restriction, in the pore space. We demonstrate the capability of our methods to distinguish different wettability states in the samples studied: water-wet, mixed-wet, and weakly oil-wet. The contact angle is spatially correlated over approximately the scale of an average pore. There is a wide distribution of contact angles within single pores. A range of local curvature is found with both positive and negative values. However, there is only a weak correlation between contact angle and curvature with lower and negative values of the curvature associated with larger contact angles (more oil-wet conditions). We observed a weak correlation between average contact angle and pore size, with the larger pores tending to be more oil-wet. Our analysis could potentially have large implications for pore-scale modeling of multiphase flow, in which methods using local curvature measurements could be directly used to calculate capillary pressures for displacement.

References:

Click here to agree

Parallel 10-E / 908

Spatiotemporally resolved PIV/SPIV velocity measurements in a MRI facility of randomly packed spheres

Thien Nguyen1; Ethan Kappes1; Mateusz Marciniak1; Stephen King1; Yassin Hassan1; Victor Ugaz1

1 Texas A&M University

Corresponding Author(s): thien.duy.ng@tamu.edu

Flows in packed beds are encountered in many engineering applications, such as solar thermal energy storages, chemical catalytic reactors, petroleum and civil engineering, magnetic refrigerators, biological tissues, and pebble-bed nuclear reactors.

Critical challenge of designing packed beds involves understanding the total pressure loss, complex flow fields, heat and mass transfer phenomena occurring within the interstitial regions. Unfortu-
nately, complex geometries and randomly connected void spaces within packed beds have hindered efforts to characterize the underlying transport phenomena.

Geometrical complexity inside of a randomly packed bed represents a challenge to experimental and computational efforts in order to construct transport models that have been previously built upon volume averages of micro-scale parameters, however, should accurately capture the flow behaviors.

Fully leveraging the advantages of this type of packed beds requires a fundamental understanding of flow topology within the randomly packed sphere beds. Multiple points or full-field measurements of flow characteristics at a high level of spatial and temporal resolutions are needed to fully map the complex flow patterns and to provide data at high spatial density to permit accurate volume averaging in the pebble bed.

Texas A&M University is conducting isothermal measurements of pressure drops, flow measurements in a randomly packed spheres experimental facility to support the research on advanced nuclear reactors sponsored by Department of Energy (DOE). The main purpose of these tests is to perform high spatial and temporal resolution measurements, and use the obtained results for code validation and model development.

In this paper, we present high-fidelity velocity measurements using Time-resolved Particle Image Velocimetry (TR-PIV) and Time-resolved Stereoscopic PIV (TR-SPIV) at the pore scales and near the wall boundary in the matching-refractive-index (MRI) facility. This approach allows us to non-invasively probe the flow within packed spheres at the microscopic scales with high temporal and spatial resolutions. Flow characteristics obtained from the TR-PIV and TR-SPIV measurements with various Reynolds numbers are presented. Results include the first- and second-order flow statistics, such as mean velocity, root-mean-square velocity and Reynolds stresses. Effects of the wall boundary and Reynolds numbers to the flow patterns are investigated. Comparisons of the mean velocities, root-mean-square fluctuating velocities, and Reynolds stress component show the increase of flow mixing and turbulent intensities within the gaps between spheres in the packed bed. Sizes of recirculation regions, however, seem to be independent versus an increase of Reynolds numbers. Finally, flow modal decompositions such as proper orthogonal decomposition (POD) and dynamic mode decomposition (DMD) are applied to reveal respectively the statistically dominant and high frequency flow modes.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 9-E / 73

Stability of saturation overshoots for two-phase flow in porous media

Martin Schneider¹ ; Rainer Helmig ¹ ; Tobias Koepl¹

¹ University of Stuttgart

Corresponding Author(s): martin.schneider@iws.uni-stuttgart.de

In this talk, we are concerned with the computational analysis of saturation overshoots for two-phase flow in porous media. In particular, it is of interest under which conditions a given saturation overshoot remains stable, while moving through a porous medium. In order to investigate this issue, we consider a decoupled and a fully coupled model, where drainage and imbibition processes are incorporated into the models by means of hysteresis models. Using the decoupled model, we estimate in the Buckley-Leverett limit the speed of the drainage and imbibition front. By these speeds, one can determine the stability of a given saturation overshoot. Moreover, they are used to compute an analytical solution for the saturation, which forms a basis for calibrating the coupled twophase flow model with respect to its boundary conditions and hysteresis parameters. Finally, we address the numerical difficulties that arise when one has to switch between an imbibition and a drainage process or vice versa.
Parallel 1-H / 430

**Stabilization of immiscible displacement in fractures by controlling aperture variability and wettability**

Zhiting Yang\(^1\); Yves Méheust\(^2\); Insa Neuweiler\(^3\); Ran Hu\(^1\); Yi-Feng Chen\(^1\); Auli Niemi\(^4\)

\(^1\) Wuhan University
\(^2\) Géosciences Rennes
\(^3\) Leibniz Universität Hannover
\(^4\) Uppsala University

**Corresponding Author(s):** zbyang@whu.edu.cn

We study immiscible fluid-fluid displacement in rough-walled fractures with a focus on the combined effect of wettability, the viscous contrast between the two fluids, and fracture surface topography on drainage patterns and interface growth. We have developed a model to simulate the dynamic displacement of one fluid by another immiscible one in a rough geological fracture; the model takes both capillary and viscous forces into account. Capillary pressures at the fluid-fluid interface are calculated based on the Young-Laplace equation using the two principal curvatures (aperture-induced curvature and in-plane curvature), while viscous forces are calculated by continuously solving the fluid pressure field in the fracture. The aperture field of a fracture is represented by a spatially correlated random field, with a power spectral density of the fracture wall topographies scaling as a power law, and a cutoff wave-length above which the Fourier modes of the two walls are identical. Results show that the model is able to produce displacement patterns of compact displacement, capillary fingering, and viscous fingering, as well as the transitions between them. Both reducing the aperture variability and increasing the contact angle (from drainage to weak imbibition) can stabilize the displacement due to the influence of the in-plane curvature, an effect analogous to that of the cooperative pore filling in porous media. Based on scaling analysis, we derive a relation between a dimensionless interface-smoothing parameter \((N_{Sm})\), defined by wettability and aperture variability, and the commonly used capillary number \((N_{Ca})\) and mobility ratio \((M)\). This relation gives a surface in the three-dimensional \((N_{Ca} - M - N_{Sm})\) parameter space, which predicts the separation of the stable and unstable displacement regimes.

**References:**


Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-A / 140

**Stabilizing Effect of Inertia on Viscous Fingering in Miscible Displacements in Porous Media**

Jinjie Wang\(^1\); Qingwang Yuan\(^2\); Long Yu\(^3\)

\(^1\) China University of Geosciences
Miscible displacements in porous media are investigated through nonlinear numerical simulations. At a relatively larger flow rate or a wider gap of Hele-Shaw cell, the inertia must be considered and its role needs to be carefully investigated. In the present study, the Reynolds number is used to quantify the inertial forces. Its effect is measured by examining the variations of viscous fingering under unfavorable viscosity ratio. It is found that the inertia has a stabilizing effect on miscible displacements compared with the cases without considering inertia. The larger the Reynolds number, the more stabilizing effect can be observed, implying the importance of consideration of inertia when analyzing miscible displacements. Moreover, we investigated the step-size time-dependent injection rate on viscous fingering for the cases with and without considering inertia. The average total amount of fluid injected is the same for constant injection rate and time-dependent rate for a certain length of time. The results show that inertia has an even stronger stabilizing effect on miscible displacement at a variable displacement rate. Meanwhile, its influence also depends on the whether the displacement starts with an injection or extraction. For different cases, the stabilizing effect of inertia is therefore quantitatively measured by analyzing the concentration field at the same time for constant injection case.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-H / 151

Stable and efficient time integration at low capillary numbers of a dynamic pore network model for immiscible two-phase flow in porous media

Author(s): Magnus Aa. Gjønestad

Co-author(s): Morten Vassvik 1; Signe Kjelstrup 1; Alex Hansen 4

1 Norwegian University of Science and Technology
2 Department of Physics, Norwegian University of Science and Technology
3 Norwegian University of Science and Technology, NTNU, Trondheim
4 NTNU

Corresponding Author(s): magnus.aa.gjønestad@ntnu.no

Numerical instabilities at low capillary numbers is a problem that has been reported for different types of pore network models [2], and first to address the issue was Koplik and Lasseter [4]. As most practical applications are in this regime, such as water flow in fuel cell gas diffusion layers and flow of carbon dioxide some distance away from the injection well in carbon dioxide sequestration, it is important to address such stability issues in a rigorous manner.

The pore network model we consider is of the type first presented by Aker et al. [1]. Since first introduced, it has been improved upon several times. With Aker-type pore network models, the numerical instabilities manifest themselves as non physical oscillations of the fluid interface positions. Some attempts to prevent these oscillations by introducing changes to the model have been made. For invasion of water in a fuel cell gas diffusion layer, Medici and Allen [5] used a scheme that allowed forward flow of water only. The price that is paid when using this approach is that interface movement is severely restricted and some dynamic effects, such as the retraction of the invasion front after a Haines jump, can no longer be resolved. Another limitation is that this scheme can only be used in transient invasion cases and studies of steady-state flow [6] cannot be performed.
As the instabilities are numerical, rigorous attempts deal with them should focus on the numerical methods, rather than introduce changes to the model. Such an approach was pursued by Joekar-Niasar et al. [3], however, for a different type of network model that the one considered here. They used a linearized semi-implicit method to achieve stabilization.

We present numerical procedures that can be used to simulate two-phase flow in porous media at low capillary numbers in a stable manner using the Aker-type pore network models. Thus, we solve the previously observed stability problems without resorting to changes in the model that restrict interface movement or prevent the study of steady-state flow. We will consider three methods, two explicit methods and a new semi-implicit method. The explicit methods are stabilized by a new time step criterion. Further, we present a thorough verification of the all three methods, confirming that they solve the model equations and exhibit correct convergence behavior, and we compare their performance.

References:


Click here to agree

Parallel 10-E / 862

Stable fingering patterns induced by an elementary hysteresis law

Ben Schweizer

1 TU Dortmund

Corresponding Author(s): ben.schweizer@tu-dortmund.de

We start from the description of unsaturated flow in porous media with the Richards’ equations. This model uses pressure and saturation as unknown variables, they satisfy one parabolic equation and one algebraic relation. The Richards’ equations provide a useful model in many situations, but they fail dramatically in the explanation of one specific experiment: When a highly saturated medium is above a very dry medium, then, driven by gravity, the fluid from the top layer enters the (initially) dry medium. In well designed experiments, it does so in the form of fingers: The fluid travels downward in thin channels. The Richards’ equations cannot explain this effect: these equations predict uniform fronts. We show that a physically motivated hysteresis model (which replaces the algebraic relation by an ordinary differential equation) can describe the effect of gravity fingering. We show some analysis for the hysteresis equations, a qualitative explanation of the fingering effect, and numerical results.
**Parallel 11-E / 180**

**Stochastic reconstruction of 3D porous media from a 2D thin slice**

**Author(s):** Yuqi Wu

**Co-author(s):** Chengyan Lin; Lihua Ren; Muhammad Jawad Munawar; Yang Wang; Yimin Zhang

**Corresponding Author(s):** wuuyu150348@163.com

Macrosopic transport properties of porous media essentially rely on the geometry and topology of their pore space. The premise of predicting these transport properties is to construct an accurate 3D pore space. A new method for reconstructing 3D porous media based on a 2D slice using the multiple-point statistics (MPS) is proposed. To validate the accuracy of the technique, Berea sandstone is chosen as the test sample. In the stochastic reconstruction process, a 2D thin section is taken as the training image and some pixels are extracted from it as the conditioning datum that must come from the centered region of a grain or pore. Then a new 2D thin section is generated using single normal equation simulation algorithm that is one of the most commonly used multiple-point statistical algorithms with the function of the simulation engine. After it, the generated image is set to the new training image and conditioning datum are anew selected from the new training image. Many 2D slices are generated by repeating the above mentioned processes. Last the stochastic porous media are generated through stacking these 2D slices. The real porous media obtained by micro-CT is used to compare the pore-space geometry and topology and transport properties with them of the reconstructed porous media. The comparison result shows that the reconstructed models are good agreement with the real model in the two-point correlation function, the pore and throat size distributions, and single- and two-phase flow permeabilities, which verifies the reliability of method.

**References:**

**Acceptance of Terms and Conditions:**

Click here to agree

---

**Parallel 1-E / 120**

**Storage and recovery of multi-component mixtures in single shale pores**

Haiyi Wu; Rui Qiao

1 Virginia Tech

**Corresponding Author(s):** ruiqiao@vt.edu

Natural gas production from shale formations has received extensive attention in recent years. While great progress has been made in understanding the adsorption and transport of single-component gas (usually CH4) inside shales’ nanopores, the adsorption and transport of multicomponent shale gas under more realistic reservoir conditions (e.g., considering CH4/C2H6 mixture) only begun to be studied. In this work, we use molecular simulations to compute the storage of CH4/C2H6 mixtures in single nanopores and their subsequent recovery. We show that, surface adsorption contributes greatly to the storage of CH4 and C2H6 inside the pores, and C2H6 is enriched over CH4. The enrichment of C2H6 is enhanced as the pore is narrowed, but is weakened as the pressure increases. These effects are captured by the ideal adsorbed solution (IAS) theory, but the theory overestimates
the adsorption of both gases. We show that the recovery of gas mixtures inside the nanopores toward a gas bath approximately follows the diffusive scaling law. The ratio of the production rate of C₂H₆ and CH₄ is close to their initial mole ratio inside the pore despite that the mobility of pure C₂H₆ is much smaller than that of pure CH₄ inside the pores. By using scale analysis and by computing the Onsager coefficients for the transport of binary CH₄/C₂H₆ mixtures inside the nanopores, we show that the strong coupling between the transport of C₂H₆ and CH₄ is responsible for the effective recovery of C₂H₆ from the nanopores.

References:

Parallel 3-E / 70

Structural Characterization of Complex Fluids in Nanopores by SANS: From Surfactant Solutions to Microemulsions

Anja Hörmann¹ ; Albert Prause¹; Bhuvenesh Bharti²; Michael Gradzielski¹; Gerhard Findenegg¹

¹ Technical University Berlin
² Louisiana State University

Corresponding Author(s): findenegg@chem.tu-berlin.de

Self-assembly of surfactants in confined geometries plays an important role in environmental, chemical and pharmaceutical technology. Adsorption of surfactants at metal oxide and other polar/charged surfaces depends primarily on the nature of their head groups: cationic surfactants exhibit high-affinity adsorption due to the interaction of the positively charged head groups with negative surface charges. Nonionic surfactants, on the other hand, exhibit low affinity adsorption isotherms due to the weak effective interaction between the hydrated head groups and hydrated surface. This difference in head group interaction with the surface causes a different evolution of surfactant aggregate morphologies at the surface. We are using small-angle neutron scattering (SANS) to study the influence of confinement on the aggregate structure of nonionic and cationic surfactants. Ordered mesoporous silica materials such as SBA-15 have favourable properties for such studies, due to the uniform size and shape of their primary pores. Studies of the aggregate morphologies of nonionic surfactants in SBA-15 have been published [1-3]. Here we will present results for the cationic surfactants DPCI and CPcI and discuss the similarities and differences in their aggregate morphologies in comparison to nonionic surfactants of the CnEm type.

The behavior of microemulsions in porous substrates is of relevance for a variety of processes, from tertiary oil recovery to soil decontamination. We will present preliminary results of a SANS study of droplet microemulsions imbibed in SBA-15, focussing on the questions if droplets of diameter greater than the pore size can enter the pores and to what extent the droplets become attached to the pore wall. Both kinds of information can be obtained by SANS measurements using a H2O/D2O solvent mixture that matches the scattering length density of the silica matrix, so that the microemulsion droplets appear against a uniform scattering background.

References:
Parallel 8-C / 720

Structural stability in synthetic rocks and metallic foams under reservoir conditions

Ignacio Figueroa\textsuperscript{1} ; Roberto Zenit\textsuperscript{1} ; ELSA DE LA CALLEJA\textsuperscript{2}

\textsuperscript{1} Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México
\textsuperscript{2} Universidad Nacional Autónoma de México

Corresponding Author(s): elsama79@gmail.com

In this talk, experimental results of structural stability of synthetic rocks and metal foams\textsuperscript{4}, subjected to reservoir conditions are presented. By controlling the injection of water and mineral oils on a confinement cell, the samples are subjected to conditions of high pressure (25KPSI) and high temperature (200°C). By means of micrography techniques the mechanical deformation of foam layers are characterized. The theoretical and experimental study of permeability and porosity in synthetic media has been studied at low pressures \cite{2,3}. However, in this work we are interested in reproducing conditions close to those of exploration and perforation for geothermal and petro physics procedures. We compare the deformation suffered by metallic aluminum foams, with the behavior of synthetic porous rocks manufactured with glass spheres. Through the theoretical model of Ahmadi \cite{4} we predict the permeability behavior in our samples. To do this we adjusted this theoretical model, taking into account the predictions of porosity and tortuosity proposed for the type of sphere used in our synthetic rocks and foams, as well as the constants of the Kozeny-Carman model \cite{5,6}. The results of our case studies are shown and stability applications are established in studies for exploration and drilling of deposits.

References:
\textsuperscript{2} D. Hernandez-Diaz, O. Chavez, A. Beltran, A. Garcia, B. Mena, and R. Zenit. Experimental study of the effect of wettability on the relative permeability for air-water flow through porous media (2017)

Click here to agree

Poster 1 / 348

Study of foam generation mechanism at the pore scale

Qingjian Li\textsuperscript{1} ; Abhishek Patel\textsuperscript{1} ; Valentina Prigiohbbe\textsuperscript{1}

\textsuperscript{1} Stevens Institute of Technology

Corresponding Author(s): qli39@stevens.edu
Foam injection into the subsurface is generally performed to improve gas mobility control during enhanced-oil recovery (EOR) and contaminated site remediation (Lake et al., 1989; Hirasaki et al., 2000; Mulligan et al., 2006). Several experiments have been conducted to study the foam generation mechanism at both the pore and continuum scales (Kovscek et al., 1994; Kam et al., 2003; Gauteplass et al., 2015; Prigiobbe et al., 2016). Pore scale experiments allow to understand the mechanism of bubble formation with a potential to help formulating constitutive equations for foam flow models improving their accuracy of prediction. However, pore scale studies have not been used to formulate foam generation rate, yet. Here, we present an experimental and modeling work on foam generation mechanism with a porous medium chip. Systematic tests at different flow conditions were performed using various chemicals to stabilize the foam, such as the surfactant, nanoparticles, and a combination of them. The pressure drop and the foam texture were monitored continuously using a pressure transducer and a high-speed high-resolution camera. We observed that to generate a foam in the presence of nanoparticles requires larger energy than when the surfactant is used to stabilize the lamellae. Possibility due to the larger critical capillary pressure for bubble rupture (Pe*) that can be reached in the presence of nanoparticles. Upon image processing, the results show that the generation rate and, therefore, the total number of bubbles increase with the injection rate, creating a more uniform bubble size distribution. We observed that nearby the gas injection the controlling mechanism of the bubble formation is snap-off, while afar from that lamella division dominates.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-H / 115

Study of the Water Saturation on a PEM Fuel Cell Cathode GDL Using a Modified Buckley Leveret Method

Author(s): Karrar Alofar

Co-author(s): Ezequiel Medici

Corresponding Author(s): ktalofar@mtu.edu

Fuel Cell is considered one of the promising technology which can be utilized in many different applications, such as stationary, transportation, and portable usage. One of fuel cell efficiency limitation is water flooding at the cathode gas diffusion layer (GDL) at high current densities or low operating temperatures. There are many different experimental and theoretical studies regarding this issue, yet the cathode GDL design is not settled. In this study, the Buckley-Leverett method is used to predict the transient water percolation throughout the GDL. In order to model the very slow water flow rates expected in a GDL, the Buckley-Leverett method was modified by including capillary pressure effects. This modified Buckley-Leverett method has the advances of predicting the transient response of the water percolation inside the GDL as well as the maximum and minimum level of water saturation. Predictions of water saturation level using the modified Buckley-Leverett method show a good agreement with existing models and ex-situ experimental observations.
References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 7-C / 652

Study of the multiple phase saturation distributions within a fracture

Meritxell Gran¹ ; Christopher Zahasky¹ ; Ryan M. Pollyea² ; Sally Benson¹

¹ Stanford University
² Department of Geosciences, Virginia Tech, Blacksburg, US

Corresponding Author(s): mgran@stanford.edu

Multiphase flow through fractured porous media has been of a great interest for decades because fractures can be the dominant flow paths in a wide range of environments, from groundwater flow and geothermal transport to fractured oil reservoirs and caprock integrity for gas and carbon storage projects. The fundamentals of multiphase flow in fractures have been studied both experimentally, mainly by means of synthetic fractures, and numerically, by assuming linear relative permeability curves. It is already known that fracture relative permeabilities are not linear functions of saturation, but still, this assumption is used due to the lack of proper relative permeability curves. A consequence of this simplification is large errors in simulated predictions and a mismatch with experimental results. With the aim of providing these crucial relative permeability curves to be used in the numerical simulations and to describe the different phase flows behavior in a fracture, multiphase core-flooding experiments are conducted in a fractured basalt rock in the context of CO2 injection. These experiments are combined with two different scan imaging techniques. X-Ray CT imaging provides information about the structure of the fracture and PET (Positron Emission Tomography) imaging shows how the fluids flow through it. The former allows us to calculate the fracture aperture distribution while from the later we obtain the phases saturation distribution. As a result, the change of relative permeability with the degree of saturation can be calculated and the nature of the multiphase fluid interactions in the fracture can be described.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-G / 501

Study on Percolation Model of Fractured Horizontal Wells in Fractal Tight Oil Reservoirs

Junqiang Wang¹ ; Yuetian Liu¹ ; Rukuan Chai²

¹ State key Laboratory of Petroleum Resources and Engineering, China University of Petroleum, Beijing, China
² Corresponding Author(s): 2279741958@qq.com, 2279749158@qq.com, rukuan_edu@163.com

Recent years, tight oil and gas has become a very important and reliable replacement for conventional energy. The porosity in tight reservoir is very small and there is a threshold pressure gradient (TPG) phenomenon and stress sensitivity in it, which make the fluid in tight reservoir hard to move and has a different employment law from the conventional reservoir, so we need a further research. Combined with the characteristics of tight reservoir, Hydraulic fracturing is the key technology for the development of tight reservoir. Traditional flowing model for multi-fractured horizontal wells
in tight oil reservoirs are mostly based on classical Euclidean geometry. However, the structure of real tight oil reservoirs is highly heterogeneous and of multiscale, and the fractal theory provides a powerful method to describe the disorder, heterogeneity, uncertainty and complexity of the complex and disordered systems. The fractal reservoir has been studied in the following aspects by making use of the Mathematical physical method, numerical calculation, computer graphics processing technology, software engineering and theoretical knowledge and application technology of the analysis method are based on the research results:

(1) Fractal geometric theory and method are good approximations to describe the complicity and we can more easily analysis all kinds of the pressure-sensitive deformable double media fractal complex reservoir relatively than others. Based on Warren-Root model, introducing fractal parameter and deformable coefficient, this thesis constructed all kinds of seepage flow mathematical models to the pressure-sensitive deformable double media fractal reservoir with the defined production or closest outside boundary when the effects caused by permeability and porosity company with the pressure change was concerned.

(2) Based on three linear flow, we established a well-testing model of fractured horizontal well in fractal reservoir, applied Laplace transform and Stehfest numerical inversion, and obtained the formulas of bottom hole pressure under the constant output. On the basis of model validation, this paper divided flow patterns and analyzed the influence of sensitivity parameters on bottom hole pressure.

(3) It is shown that there mainly exists wellbore storage, transition flow, pseudo-linear flow, pseudobilinear flow and boundary flow and at the same time fractals dimensions has a great influence on the bottom hole pressure.

References:


Parallel 10-H / 160

Study on SAV scheme in Diffuse Interface model for the multiphase fluid system with the Peng-Robinson equation of state

Author(s): Tao Zhang¹ ; Shuyu Sun¹
Co-author(s): Yuze Zhang ²

¹ King Abdullah University of Science and Technology
² The Hong Kong Polytechnic University

Corresponding Author(s): tao.zhang.1@kaust.edu.sa

Modeling and simulation of multiphase flow and transport in underground porous media is an essential component in many scientific and engineering applications. Now, more and more focus has been paid on the Diffuse Interface models, which describes the interface as a continuum three-dimensional entity separating the two bulk single phase fluids. Realistic equation of state (e.g. Peng-Robinson equation of state), has been proved to be a more accurate choice to model the interface tension, compared to a simple double-well potential. To handle the unconditionally energy stable requirement, a method called invariant energy quadratization (IEQ) is proposed. This approach allows us to construct a linear and unconditional energy stable
scheme. However, the coefficients in this method are variables, which hinders the application of the fast fourier transformation method. To overcome it, a stabilized predictor-corrector approach is proposed and introduced, which is also called scalar auxiliary variable (SAV) scheme, to construct schemes which are second –order accurate, easy to implement, fast to divergence and maintaining the stability of the first-order stabilized schemes.

In this paper, the coupled model combined with diffuse interface model and Peng-Robinson equation of state is applied to describe the phenomenon around the interface. In this scheme, the Helmholtz free energy is used as the kernel, and a gradient term is added as well. The Cahn-Hilliard equation is the H-1 gradient flow of the total free energy. Unlike the Allen-Cahn equation, the Cahn-Hilliard itself can preserve the total mass because the function is based on the mass conservation law. As a result, if we treat the equilibrium in the fourth order form, we will not need to deal the Lagrange multiplier and we can get a Cahn-Hilliard equation-like model as

$$n_t + \sum_{j=1}^{M} c_{ij} \Delta^2 n_j = \Delta \mu_0$$

Figure 2: Cahn-Hilliard equation-like model

The main idea of the SAV scheme is to introduce the following term, the problem transforms to

$$\begin{cases}
    n_t = \Delta \mu; \\
    \mu = -C \Delta^2 n + \frac{r}{\sqrt{E_p + C_0}} \Delta \mu_0(n); \\
    r_t = \frac{1}{2 \sqrt{E_p + C_0}} \int_{\Omega} \mu_0(n) n_t dx,
\end{cases}$$

Figure 3: enter image description here

We first simulate the separation of two phases of isobutene (nC4) at the temperature around 250K to 350K. Figure 3 shows the evolution of the solution of the fourth-order model.

Figure 4: Fig.3

We can see that a gas-liquid interface is formed around each liquid drops and the shape of the single drops become circle at the early stage. Then, the gas-liquid interface of each drops touch each other and these 4 drops start to mix together. Finally, a unit one is formed at the center of the whole
domain. Figure 4 illustrates the energy dissipation trend during the evolution history and the mass conservation property.

![Graph showing energy dissipation trend](image)

**Figure 5: Fig.4**

Figure 5 shows the comparison of the surface tension obtained by the numerical experiment and the data from laboratory and our work meets the experiment data very well.
Figure 6: Fig.5

To show the numerical efficiency of such scheme, a 3D simulation on a 200x200x200 mesh is conducted and we can still get reasonable result.
Studying surfactant loss at rock-liquid interface using Quartz Crystal Microbalance

Naveen Kumar¹ ; Marcel Bus¹ ; Esther van den Pol² ; Johannes van Wunnik² ; Ernst J. R. Sudhölter¹

¹ TU delft
² Shell Global Solutions International B.V.

Corresponding Author(s): n.kumar-2@tudelft.nl

Surfactant flooding is one of the mechanisms used to enhance oil recovery from oil reservoirs. Surfactants mainly reduce interfacial tension, increase oil mobility thus allowing better displacement of oil by injected water. One of the main challenges in this process is the loss of surfactant due to adsorption on reservoir rocks. The first adsorbed layer of surfactant is mostly governed by electrostatic attraction. Once this first adsorbed patch forms on the surface, a second layer of surfactant

Figure 8: Fig.7
may be adsorbed by surfactant tail-tail hydrophobic interactions at high surfactant concentrations. Both these interactions would be affected by the salt type, salt concentration and pH of the injected solution. In this study, adsorption of anionic surfactants is investigated on negatively charged silica and positively charged calcite and alumina surfaces under various brine conditions. Further, we also check the efficiency of a polyelectrolyte solution as sacrificial agent to minimise the surfactant adsorption. We use QCM and surface tension measurements to study the same. Both QCM and surface tension measurements reveal the extent of surfactant adsorption. In case of QCM, the change in frequency of quartz crystal gives information about adsorbed mass while in case of surface tension (γ) measurements, change in γ tells about the concentration change of surfactant in the bulk and hence indirectly about the surfactant adsorption. In case of negatively charged silica surface, the anionic surfactants adsorb readily in presence of divalent ions, while there is very slight or negligible adsorption in presence of only monovalent ions. Hence the adsorption is mediated via cation bridging mechanism. In case of alumina (positively charged below pH 9), we see significant adsorption even in absence of divalent ions. This occurs due to direct electrostatic attraction between the negative polar head group of surfactants and the positive alumina surface. The surfactant adsorption can be reduced by a pre-flush of anionic polyelectrolyte which has stronger binding affinity for the surface compared to surfactants. The strongly adsorbed poly-electrolyte repels similarly charged surfactant molecules and hence reduces surfactant adsorption. Similar trends are also observed with the surface tension measurements. The pre-flush of anionic polyelectrolyte reduces the surfactant adsorption on the sandstone powder, which leads to higher bulk concentration of surfactant and hence a smaller value of surface tension. We discuss our findings in the context of improving the efficiency of the alkaline surfactant polymer flooding process.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-E / 743

Supercritical Methane Sorption on Organic-Rich Shales from Sichuan Basin, China

Feng Yang1; Boyu Hu1

1 China University of Geosciences, Wuhan

Corresponding Author(s): fengyang@cug.edu.cn

Fine-grained sedimentary rocks, such as mudstones and shales, contain abundant nanometer- to micrometer-sized pores. These narrow pores create intense fluid-rock interaction that may lead to complicated fluid storage and transport process. Concerns about the accurate evaluation of gas content and diffusion kinetics have led to many experimental studies about gas sorption on shales. However, data on high-temperature high-pressure sorption isotherms of shales are still scare. In particular, the burial depth of the Paleozoic shales in the Upper Yangtze region of China is mostly in a range of 2000–4000 m, which indicates that the temperature and pressure of shale reservoirs are in the range of 60–120 °C and 20–40 MPa. Experimental techniques employed in obtaining sorption data have to be optimized and at the same time the measuring conditions have to be extended to in-situ conditions of deep shales while many published sorption data are limited to moderate pressures and temperatures. In this work, high-temperature high-pressure sorption data for methane on shales from Sichuan Basin have been obtained at 30–120°C and pressures up to 25 MPa using a specially designed two-temperature-zone manometric setup. Dubinin-Polanyi potential theory was modified to extend to supercritical gas sorption over wide temperature and pressure ranges. A modified adsorption potential method was proposed to calculate the characteristic curves for supercritical gas sorption, and then a rigorous function from the supercritical Dubinin-Astakhov equation was also developed to describe the modified characteristic curve. Furthermore, the physical meaning of characteristic curve has been elucidated by comparing characteristic curves of different kinds of shales and clay minerals. The measured excess sorption isotherms of shales follow the physisorption trend of decreasing amounts of methane adsorbed with increasing temperature. Characteristic curves of methane on...
shales at 30–120°C were calculated using a new expression of adsorption potential. It is found that if the thermal expansion of adsorbed phase is considered, these modified characteristic curves are temperature-invariant. The characteristic curve equation is capable to predict methane sorption at other temperatures based on the easily tested isotherm at room temperature. Using the sorption isotherm and characteristic curve equation at 30°C, the predicted isotherms at 120°C agree well with experimental data. The modified characteristic curves comprehensively characterize the available pore space for sorption and the affinity of methane molecules. The later stage of the modified characteristic curves (limited adsorption volume) is mainly controlled by the available pore space provided by organic matter and clay minerals. The limiting adsorption volume of shales in the gas window is larger than shales in the oil window with the same TOC content. The initial stage of the characteristic curves reflects the affinity of methane molecules for sorption on organic matter. According to the characteristic curves, shales in the gas window show higher affinity than shale in the oil window and clay minerals, though the clay minerals may provide comparable adsorption volume. The sorption characteristic energy shows a parabolic-like shape with a minimum approximately around Req =1.1%, which are related with the evolution of porosity of shales.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-G / 84

Superfluid and quantum turbulence in porous media

Cyprien Soulaine\(^1\); Michel Quintard\(^2\); Bertrand Baudouy\(^3\); Rob van Weelden\(^4\)

\(^1\) Stanford University
\(^2\) Institut de Mécanique des Fluides de Toulouse
\(^3\) CEA
\(^4\) CERN

Corresponding Author(s): cyprien.soulaine@gmail.com

Below 2.17 K, helium no longer behaves as a classical fluid: it has almost no viscosity and a high effective thermal conductivity that is used to cool superconducting devices such as the Large Hadron Collider’s magnets. Beyond a critical velocity, quantum turbulence arises and complex flow patterns appear.

We developed a numerical tool to simulate helium superfluid flow in porous media at the pore-scale. We were able to reproduce and explain, for the first time, interesting and unexpected experimental observations about thermal counterflow of He II past a cylinder reported ten years ago. Eddies are generated through a complex transient process that involves the friction of the normal fluid species with the solid walls and the mutual friction between the superfluid and normal species. The vortices remain in single pores and eddies spanning over several pores are not observed suggesting that a Darcy-Forchheimer type law can be used to model quantum turbulence in porous media.

References:

Cyprien Soulaine, Michel Quintard, Hervé Allain, Bertrand Baudouy, Rob Van Weelden, A PISO-like algorithm to simulate superfluid helium flow with the two-fluid model, Computer Physics Communications 187 (2015)


Click here to agree

Poster 3 / 464
Surface complexation modeling of arsenic mobilization from goethite: Interpretation of in-situ experiments in a sedimentary basin of Inner Mongolia, China

Author(s): Lucien Stolze
Co-author(s): Di Zhang ; Huaming Guo ; Massimo Rolle

1 School of Water Resources and Environment, China University of Geosciences, Beijing, China
2 Technical University of Denmark

Corresponding Author(s): lucst@env.dtu.dk

Sorption competition onto Fe-(oxyhydr-)oxides surfaces is a well-known mechanism controlling the release and mobility of arsenic (As) in subsurface (Dixit & Hering, 2006). Over the last decades, surface complexation models (SCMs) have been implemented to model interactions between sorbants and mineral-oxides surfaces by considering the thermodynamic properties underlying complexation and electrostatic interactions (Goldberg, 1992). However, SCMs development are typically based and/or applied on well-controlled laboratory experiments with simple aqueous systems rather than complex environmental groundwater conditions.

In this study, we present and compare conceptual and numerical modeling approaches developed to quantitatively interpret in-situ experiments that consisted in monitoring the temporal change of adsorbed-As concentration by incubating As-loaded goethite coated sand in the groundwater (Zhang, et al., 2017). Reactive transport models were developed using the Iphreeqc model coupling the geochemical code PHREEQC and MATLAB (Muniruzzaman & Rolle, 2016). The two surface complexation modeling approaches available in PHREEQC, the diffuse double layer (DDL) and the charge-distribution multisite complexation (CD-MUSIC) models (Hiemstra & Van Riemsdijk, 1996), were applied to simulate sorption competition assumed to be the only geochemical process leading to the release of As from goethite. Model parameters were calibrated through inverse modeling in order to simulate experimental results. Whereas a satisfying agreement with the measured As-adsorbed concentrations was obtained, the role of the aqueous species in the As desorption significantly differs between the predictions of the DDL and the CD-MUSIC models.

References:

Click here to agree

Poster 3 / 694

Surface roughness and deformation effects on the thermal characterization of granular porous media

Roohollah Askari ; S. Hossein Hejazi ; Muhammad Sahimi

1 Department of Geological and Mining Engineering and Sciences, Michigan Technological University
2 Subsurface Fluidics and EOR Laboratory, Chemical and Petroleum Engineering, University of Calgary
3 Mork Family Department of Chemical Engineering and Materials Science, University of Southern California
Corresponding Author(s): moe@usc.edu

Heat conduction in porous materials is of great interest for geological and engineering studies including geothermal reservoirs, insulating layers, composite materials, to name a few. In the absence of flow, thermal energy is transferred through the constituting materials of porous media with different capabilities in conducting heat. Thus, the structure of phase boundaries, the contact area between the grains in a granular porous medium for example, becomes essential in the accurate modeling of heat transfer. In the present study, we adopted a fractal contact model of rough surfaces that is based on the Weierstrass and Mandel function (W-M model) to estimate roughness deformation and contact areas in granular porous media. The roughness deformation is a function of roughness fractal parameters, grains’ Young modulus, and compressing pressure. Heat conduction in a packing of particles under compressive pressure is studied. It is revealed that grains with smoother surfaces and lower Young’s moduli experience the highest deformation for a given compressing pressure. Effective thermal conductivity is an increasing function of compressing pressure where the effect of compressing pressure is more noticeable in media with the high ratio of thermal conductivity of solid to that of fluid.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-F / 767

Surfaces of hyperbolic-parabolic transition in the problem of flow with variable number of phases through porous media

Mikhail Panfilov

1 Institut Elie Cartan - Université de Lorraine & Institut d’Alembert - Sorbonne Universités

Corresponding Author(s): michel.panfilov@dalembert.upmc.fr

An interface of phase transition is a macroscopic surface that separates the domain occupied by a single-phase gas or liquid from another domain occupied by two-phase gas-liquid mixture. In classical fluid dynamics an example of such a surface is the boundary of a cloud or a spray in the air. In porous media, this corresponds to the injection of miscible gas in an oil reservoir, which creates the zone of single-phase gas near the injection well, another zone of single-phase oil near the producing well, and a two-phase zone between them. Two mobile boundaries of the two-phase zone are the surfaces of phase transition. To model such systems, the method of negative saturations has been developed, which enables us to describe the overall fluid in all zones by a uniform system of extended two-phase equations and to solve it by direct numerical simulation without applying any special technique of front tracking. In this method the overall fluid is assumed to be pseudo two-phase. The extended system of equations is obtained from the principle of equivalence between the two-phase and single-phase flow.

Such an extended model of two-phase flow can be reduced to a single equation of nonlinear kinematic waves with respect to the gas saturation. It contains some non-classical terms like the extra-diffusion (the diffusion of phase saturation). This equation is parabolic in the subdomains that correspond to the true single-phase fluid, and hyperbolic in the zone of the true two-phase flow. Then a physical surface of phase transition is equivalent to the mathematical interface of transition between hyperbolicity and parabolicity (HP-transition). It is possible to show that such an interface represents a strong discontinuity of the solution (HP-shocks). We develop the extended Hugoniot-Rankine conditions and the entropy conditions for them. For one-dimensional Riemann problem, a graphical technique has been developed, which enables us to calculate the exact velocity of a HP-shock and the saturation behind and ahead of it. For numerical simulation of the extended two-phase model with HP-transition, two types of regularization are analysed: the introduction of small capillary or fictitious diffusion and the Kirchhoff regularization. Several examples of the solution are shown.
References:
Click here to agree

Poster 3 / 894

Swelling and fracture of ionized, highly deformable hydrogels.

Jacques Huyghe¹ ; Cong Yu² ; Jingqian Ding² ; Eanna Fennell³

¹ University of Limerick
² Eindhoven University of Technology

Corresponding Author(s): jacques.huyghe@ul.ie

Many technical materials, biological tissues and living cells are ionized porous media. Under changes of osmotic boundary conditions, these ionized gels respond by swelling to many times their own volume. As the macromolecular network of the gels has limited strength, fracture propagation may occur. Modelling of 3D finite swelling and subsequent fracture requires very careful modelling. Regular u-p formulations of swelling often fail to converge at the low stiffness considered. Our group developed a mixed hybrid finite element model of swelling of gels. Superior robustness is demonstrated. Fraction propagation under finite deformation is modelled including fluid flow within the crack and exchange of fluid between crack and gel. Comparison with experiments on fracture propagation demonstrate that the model reproduces staccato propagation of fracture in gel.

References:

Click here to agree

Poster 2 / 225

Synthesis and characterisation of B-substituted nanoporous carbons with high energy of hydrogen adsorption.

Author(s): Katarzyna Walczak¹
Co-author(s): Lucyna Firlej ² ; Bogdan Kuchta ³

¹ Laboratoire Charles Coulomb, University of Montpellier, France
² Charles Coulomb Laboratory, University of Montpellier
³ Laboratoire MADIREL

Corresponding Author(s): katarzyna.walczak@umontpellier.fr

The world is running out of fossil fuels and the products of their burning in air (mostly CO2) have already impacted global climate. Today it is clear that in near future we need to convert the global energy economy towards cleaner and renewable fuels (like hydrogen). However, to efficiently store hydrogen at ambient temperature and not too high pressures, we need to develop the hydrogen sorbent with simultaneously optimized specific surface and adsorption energy.
Here we report the first studies of the potential effectiveness of arc-discharge procedure to synthetize nanoporous, carbon based sorbents with characteristics required for hydrogen storage in vehicular applications. The arc-discharge, successfully used in the past to synthetize fullerenes and nanotubes, provides a relatively easy way to incorporate heteroatoms into pure carbon structures. Therefore we have assumed that we can adjust the synthesis parameters to prepare other graphene-based structures, with a variety of shapes, sizes, and interconnections between graphene fragments.

The properties of first boron-substituted carbons obtained by this method are promising: the prepared carbon soot contains a variety of organized, graphene based structures, and the HRTEM and NMR study confirm the presence of boron nanoclusters, partially incorporated into graphene layers. The energy of hydrogen adsorption is the highest ever observed experimentally in carbon-based sorbents: at least 10% of adsorption sites adsorb hydrogen with the energy higher than 6.5 kJ/mol, and the strongest adsorption occurs with energy higher than 10 kJ/mol. These values are significantly larger than hydrogen adsorption energy in activated carbons (~4.5 kJ/mol). However, the specific surface of as-prepared samples is low (~200 m²/g), even after thermal activation. Therefore the samples are currently activated chemically (with KOH); this procedure should increase the surface accessible for adsorption by one order of magnitude.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-C / 370

System Reduction of Discrete Fracture Network Simulations Using Graph-Based Methods

Jeffrey Hyman¹ ; Aric Hagberg¹ ; Gowri Srinivasan¹ ; Hari Viswanathan¹ ; Shriram Srinivasan¹

¹ Los Alamos National Laboratory

Corresponding Author(s): jbyman@lanl.gov

Discrete fracture network (DFN) models explicitly use fracture geometry and network topology to simulate flow and transport through fractured systems. Recent advances in high performance computing have opened the door for flow and transport simulations in large explicit three-dimensional DFN. However, this increase in model fidelity and network size comes at a huge computational cost because of the large number of mesh elements required to represent thousands of fractures (with sizes that can range several orders of magnitude, from mm to km). We will discuss coarse scale graph representations of DFN and how they can be used to exploit geometric and topological properties of DFNs to perform system reduction without loss of accuracy for key quantities of interest. In particular, different graph-representations of DFN models and how they can be used to reduce the computational burden associated with DFN models will be demonstrated.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 2 / 45

THERMOSTABLE NANOPOROUS CYANATE ESTER RESINS NEWLY DESIGNED BY USING IONIC LIQUIDS AS POROGENS

Daniel Grande² ; Alina Vashchuk² ; Alexander Fainleib³ ; Olga Starostenko³ ; Olga Grigoryeva³ ; Sergiy Rogalsky³ ; Thi-Thanh-Tam Nguyen⁵
Porous polymeric materials have a large variety of applications in many areas as highly selective membranes, selective adsorbents and filters, porous electrodes for fuel cells, sensors or insulators, etc. High crosslink density Cyanate Ester Resins (CERs) – also known as polycyanurates (PCNs) – are commonly used in aerospace applications and electronic devices as thermostable polymer matrices. Ionic liquids (ILs) are defined as organic/inorganic hybrid salts with melting points below or equal to 100°C. ILs have attracted widespread interest in polymer science, due to their versatile properties, such as negligible saturated vapor pressure, wide liquid-state temperature range, incombustibility, high electrical conductivity, high thermal stability, and stability to oxidation [2-3].

In the present work, novel nanoporous film materials of thermostable CERs were generated by polycyclotrimerization of dicyanate ester of bisphenol E in the presence of varying amounts (from 20 to 40 wt. %) of an ionic liquid (IL), i.e. 1-heptylpyridinium tetrafluoroborate([HPyr][BF4]), followed by its quantitative extraction after complete CER network formation. The completion of CER formation and IL extraction were assessed using gel fraction content determination, FTIR, 1H NMR, and energy dispersive X-ray spectroscopy (EDX). The morphology and porosity features, such as pore diameters and pore size distributions of the samples, were estimated by SEM and DSC-based thermoporometry. SEM micrograph demonstrated the formation of nanoporous structures after IL removal from CER networks, thus showing the effective role of IL as a porogen. Pore sizes varied from ~20 to ~180 nm with an average pore diameter of around 45-60 nm depending on the initial IL content. The thermal stability of thenanoporous CER-based films was investigated by thermogravimetric analysis (TGA). The TGA curves showed high thermal stability of the nanoporous films obtained with a decomposition temperature onset near 300°C.

It should be stressed that the synthesis of CERs in the presence of IL was carried out without using any additional solvent or specific catalyst, the ionic liquid being highly thermostable and potentially being utilized repeatedly.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-B / 44

TUNING PORE MORPHOLOGY AND FUNCTIONALITY IN SOFT POROUS MATERIALS

Daniel Grande

1 Institut de Chimie et des Matériaux Paris-Est
Corresponding Author(s): grande@icmpe.cnrs.fr

Over the last decade, the generation of organic porous (nano)materials with tunable pore sizes and desired functionalities has been the subject of increasing attention in materials science. Interest in such porous frameworks originates from the large variety of applications in which they are involved, e.g. size/shape-selective nanoreactors, monoliths for advanced chromatographic techniques, nanofiltration membranes, high specific area catalytic supports, as well as 3-D scaffolds for tissue engineering.

This lecture examines the scope and limitations of three different approaches to porous polymers with controlled porosity and functionality at different length scales. The first approach relies on the synthesis of polystyrene-block-poly(D,L-lactide) diblock copolymers with functional groups at the junction between both blocks, followed by their macroscopic orientation, and the subsequent selective removal of the polyester block to afford ordered nanoporous materials with channels lined with chemically accessible functionalities (e.g., COOH, SO3H, SH, COH) [1-4]. The second strategy entails the preparation of biocompatible doubly porous crosslinked polymer materials through the use two distinct types of porogen templates, namely a macroporogen in combination with a nanoporogen. To generate the macroporosity, either NaCl particles or fused PMMA beads are used, while the second porosity is obtained by using a porogenic solvent [5]. Alternatively, a straightforward and versatile methodology for engineering doubly porous polymers is implemented through a thermally induced phase separation process [6]. Finally, 3-D macroporous scaffolds based on biodegradable polymers have been engineered by electrospinning to generate nanofibrous biomaterials that mimic the extracellular matrix [7,8]. The potentialities afforded by these approaches will be addressed, and some typical applications of the resulting porous materials will be illustrated.

References:

Click here to agree

Parallel 7-D / 799

The Control of Wettability for a Micror-Fluidic Channel using Electrokinetic Technique and its Effect on Externally Measured Pressures

Author(s): Xuhui Zhou thoughtful research assistant
Co-author(s): David Nolte ; Laura Pyrak-Nolte

1 Purdue University

Corresponding Author(s): zhou412@purdue.edu

The hysteretic relationship between capillary pressure (Pc) on saturation (S) has been shown to be a projection of a higher-dimensional surface that depends on interfacial area per volume (IAV) as the additional state variable. Most studies that validate the capillary-pressure-saturation-IAV relationship are performed on 2D micro-models or cores where scanning is performed in pressure
and not in saturation. We have developed an EWOD technique (electro-wetting on dielectric) to internally manipulate fluid saturation to determine the effect on externally measured pressures. Applying electric fields to electrolytic fluids changes the contact angle among the fluids and the solid. For a parallel-plate electro-wetting set-up, the pressure difference is given by gsl (cosq(EW - cosqEW )/d’, where d’ is the aperture, qEQ and qEW are the contact angles before and after the application of voltage, V, and gsl is the interfacial tension between the solid and liquid phases. This pressure difference enables direct control over internal fluid distributions. The contact angle reverts to the original value when V = 0.

A sealed micro-model with Electro-Wetting on Dielectric (EWOD) electrodes was fabricated using a PDMS wedge-shaped channel with an entrance width of 0.5 mm and an exit width of 2 mm. The channel length was 4 mm, and had a depth of 0.9 mm. The PDMS channel was attached to an aluminum plate that served as the ground electrode. An ITO slide coated with PDMS formed the high voltage electrode and was used to seal the micro-model. X-ray Micro-CT scans showed that the contact angle between electrodes changes from from -110° (non-wetting) to ~70° (wetting) for an applied voltage of 318 V AC.

By applying voltage to the wedge-shaped micromodel, with the inlet and the outlet opened to the atmosphere, the externally measured capillary pressure remained constant even though the fluid-air interface moved and the saturation increased. A comparison of hysteresis loop with/without voltage exhibits a difference of ~20 Pa in the drainage scan while almost the same in the imbibition scan. For a closed system, the externally measured change in capillary pressure was ~30 Pa and the saturation in the channel increased. To explore the effect of roughness, micro-model with different roughness steps were fabricated. With rough channels, pinning was observed. EWOD provides method to assess the contributions of wettability to the fundamental physics of immiscible fluids in analog porous media.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 819

The Effect of Original and Initial Saturation on Residual Nonwetting Phase Capillary Trapping Efficiency

Dorthe Wildenschild\footnote{Oregon State University} ; Elizabeth Harper Kimbrel\footnote{Oregon State University} ; Ryan Armstrong\footnote{Oregon State University}

Injection of supercritical carbon dioxide (CO2) into geological formations is used for both atmospheric greenhouse gas reduction (climate change mitigation) and enhanced oil recovery. In an effort to fully understand CO2 trapping efficiency, the capillary trapping behaviors that immobilize subsurface fluids were analyzed at the pore-scale using pairs of proxy fluids representing the range of in situ (supercritical) nonwetting and wetting fluids. The pairs of fluids were cycled through imbibition and drainage processes using a flow cell apparatus containing a sintered glass bead column. Computed x-ray microtomography (microCT) was used to identify immobilized nonwetting fluid volumes after imbibition and drainage events.

From the images, the trapped residual (post-secondary imbibition) nonwetting phase was spatially correlated to both the original (post-primary imbibition) and the initial (post-primary drainage) nonwetting phase; relationships referred to as the original saturation dependence (So-dependence) and initial saturation dependence (Si-dependence), respectively. Statistically significant trends of decreasing So- and Si-dependence with increasing wetting and nonwetting fluid phase viscosities were observed. This finding implies that the amount of CO2 injected and ultimately trapped is dependent on the nonwetting phase (e.g. oil or gas) already present in the formation, as well as on the manner in which supercritical CO2 is initially injected.

References:

Acceptance of Terms and Conditions:
Parallel 4-C / 651

The Effects of Chemomechanical Processes on Limestone Weathering Rates

Lawrence Anovitz¹; Timonthy Prisk²; Simon Emmanuel³; Michael Cheshire¹; Juliane Weber¹; Susan Brantley⁴; Markus Bleuel²; Jan Ilavsky⁵; David Mildner⁶; Cedric Gagnon⁶

¹ Oak Ridge National Laboratory
² Nist Center for Neutron Research
³ Hebrew University, Jerusalem
⁴ Pennsylvania State University
⁵ Advanced Photon Source, Argonne National Laboratory
⁶ NIST Center for Neutron Research

Corresponding Author(s): anovitzlm@ornl.gov

Dissolution within porous media is a critical process in many environmental and geological settings. The formation and evolution of soils, rocks, and landscapes (Buhmann and Dreybrodt, 1985; Brantley, 2008; Jin et al., 2010), efficiency of carbon capture in geological reservoirs (Matter and Kelemen, 2009), and the weathering of man-made structures are all highly dependent on the rates at which minerals dissolve. However, the factors governing dissolution in geological media are not yet well understood. In general, rock dissolution rates are governed by fluid composition, fluid flow rates, and the surface area of the mineral–fluid interface (Lasaga, 1998). As a surface becomes rougher, the surface area in contact with a reactive fluid increases, and it is therefore often assumed that rough surfaces dissolve more rapidly than smooth surfaces (Fischer and Lüttege, 2007). However, a number of studies have shown a complex relationship between roughness and reactivity (e.g., Anbeek, 1992; Gautier et al., 2001). Emmanuel and Levenson (2014) found that erosion rates in fine-grained micritic limestone blocks are as much as two orders of magnitude higher than rates estimated for coarse-grained limestones. AFM imaging suggested this is the result of rapid dissolution along microscale grain boundaries, followed by mechanical detachment of tiny particles from the surface. Such chemo-mechanical processes may be the dominant erosional mode for fine-grained carbonate rocks in many regions on Earth. This erosion extends to the micron scale, and grain detachment can be a crucial mechanism controlling denudation rates in carbonate terrains.

In order to better understand this weathering process we undertook a series of experiments looking at the weathering of carbonates. 5/8” x 5/8” cores of four limestones (Netzer, Shiuvti, Carthage Marble, Texas Cream) were exposed to flowing water at 30°C and several pH values to mimic the weathering process. Annular Cd masks of stepped sizes, and small beam stepped locations analyses, were used to analyze the weathering structure by (U)SANS and (U)SAXS as a function of distance from the edge. SEM analysis was also used to look at the pore structure and surface weathering. The results, both in terms of core/rim variations and pore size dependence, were found to be strongly dependent on initial permeability and rock structure, as well as time and pH.

References:

Click here to agree
Parallel 9-E / 536

The Effects of Dynamic Capillary in Modeling Saturation Overshoot during Infiltration

Author(s): Luwen Zhuang
Co-author(s): S.M. Hassanzadeh

1 Utrecht University

Corresponding Author(s): l.zhuang@uu.nl

The typical characteristic of a thin porous layer is that its thickness is much smaller than its in-plane dimensions. A stack of thin porous layers creates contact interfaces, whose properties are quite different with thin layers. Determining the hydraulic properties is essential to understand and model fluid flow in thin porous media. The validity of classical methods in thin porous media is doubtful, because of the huge differences between thin porous media and normal porous media.

In this work, we constructed a relatively simple experimental setup for measuring the hydraulic properties for a stack of thin porous layers. We performed a series of experiments using the uniform-gradient-flow method. Both saturation and water pressure values were measured for different thicknesses of layers.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 1 / 673

The Flow of a Shear-Thinning Fluid in a Geological Fracture

Clément Roques, Yves Méheust, Tanguy Le Borgne, John Selker

1 ETH Zürich
2 Géosciences Rennes
3 University of Rennes
4 Oregon State University

Corresponding Author(s): yves.mehheust@univ-rennes1.fr

Subsurface flow processes involving non-Newtonian fluids play a major role in many engineering applications, from in-situ remediation to enhanced oil recovery. The fluids of interest in such applications (i.e., polymers in remediation) often present shear-thinning properties, i.e., their viscosity decreases as a function of the local shear rate. We investigate how fracture wall roughness impacts the flow of a shear-thinning fluid. Numerical simulations of flow in 3D geological fractures are carried out by solving a modified Navier-Stokes equation incorporating the Carreau viscous-shear model. The numerical fractures consist of two isotropic self-affine surfaces which are correlated with each other above a characteristic scale (Meheust et al., 2003). Perfect plastic closing is assumed when the surfaces are in contact. The statistical parameters describing a fracture are the standard deviation of the wall roughness, the mean aperture, the correlation length, and the fracture length, the Hurst exponent being fixed (equal to 0.8). The objective is to investigate how varying the correlation length impacts the flow behavior, for different degrees of closure, and how this behavior diverges from what is known for Newtonian fluids. The results from the 3D simulations are also compared to 2D simulations based on the lubrication theory, which we have developed as an extension of the Reynolds equation for Newtonian fluids. These 2D simulations run orders of magnitude faster, which allows considering a significant statistics of fractures of identical statistical parameters, and therefore draw general conclusions despite the large stochasticity of the media.
Parallel 5-G / 260

The Formation of Microemulsion at Flow Conditions in Rock

Steffen Berg1; Evren Unsal1; Maja Ruecker2; Willem-Bart Bartel3; Niels Brussee1; Ab Coorn1; Anne Bonnin4

1 Shell Global Solutions International B.V.
2 Imperial College London
3 Utrecht University
4 Swiss Light Source, Paul Scherrer Institute

Corresponding Author(s): steffen.berg@shell.com

Surfactant flooding is a chemical enhanced oil recovery (cEOR) technique where a low concentration of surfactant is added to the injection water. The surfactant reduces the oil/brine interfacial tension which, in return, increases the capillary number favoring the viscous mobilization of (capillary) trapped oil. In order to reduce the residual oil saturation significantly, ultra-low interfacial tension (<10-2 mN,m-1) between crude oil and aqueous phase is required. That is achieved by employing surfactants that solubilizes the oil and form a microemulsion phase. How low interfacial tension can become depends on the phase behaviour of the surfactant/oil/water system which is often studied with equilibrium phase behaviour tests. However, oil recovery is a dynamic process, and microemulsion formation occurs in situ over different time and length scales depending on the flow and porous medium characteristic.

In this study, we investigated in-situ formation of microemulsion and mobilization production of oil by solubilization in the core samples. The aqueous solution of an EOR surfactant was injected into the core sample after the waterflood to solubilize the remaining oil. The surfactant was an internal olefin sulfonate (IOS), and had affinity to the oil phase (n-decane); in situ microemulsion formation occurred. The oil phase was doped with iodo-decane as contrast agent, which allowed visualization of the oil-and emulsion phases using X-ray computed micro-tomography technique. The resolution was sufficient to visualize pure and emulsified oil within individual pores. Image analysis of the scans showed that the emulsification during flow took place at shorter time scales than what was observed at static conditions. These results were consistent with findings of micromodel experiments.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 773

The Impact of Precipitation Scenarios on the Characteristics of Porous Media: Numerical Simulation vs Experiments

Nariman Mahabadi1; Hamed Khodadadi Tirkolaei1; Vinay Krishnan4; Leon van Paassen1

1 Arizona State University

Corresponding Author(s): nmahabad@asu.edu
Several biological processes have been developed in the recent years in which the hydro-mechanical soil properties can be modified by precipitating calcium carbonate. Microbial and enzyme induced carbonate precipitation (MICP and EICP) have gained interest in potential biological processes to improve the mechanical properties of the soil by precipitating calcium carbonate, which forms cementing bonds between soil particles. However, the formation of inter-particle cementation also alters the porosity and connectivity of the pores and the hydrodynamics of the porous media. In this study, a computational algorithm is developed using a pore network model generated based on the initial grain size distribution and void ratio of a sand sample. The effect of the initial conditions such as hydrolysis rate and particle/pore characteristics on the carbonate precipitation behavior is studied and employed into the numerical algorithm. In addition, the effect of different resulting precipitation patterns such as contact binding, grain coating and pore filling on the fluid flow, permeability, water retention characteristics and pore size distribution of the bio-cemented soil samples are simulated using the pore network model. The numerical results are compared to the experimental hydraulic conductivity and soil water characteristics measurements of the EICP treated soil samples.

References:

Acceptance of Terms and Conditions:

Click here to agree

Invited 1 (Room D) - Ralf Seemann / 1113

**The Role of Local Instabilities in Fluid Invasion into Permeable Media Studied by in situ X-Ray Microtomography**

**Author(s):** Ralf Seemann

Co-author(s): H. Scholl ²; K. Singh ²; W. Li ²; P. Shakeri ²; M. Di Michiel ³; M. Scheel ³; M. Brinkmann ²; S. Herminghaus ⁴

¹ Saarland University/MPIDS

² Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany. Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

³ European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble, France

⁴ Max Planck Institute for Dynamics and Self-Organization, D-37073 Göttingen, Germany

**Corresponding Author(s):** r.seemann@physik.uni-saarland.de

Considering the paradigmatic case of random piles of spheres, fluid front morphologies emerging during slow immiscible displacement with a global front velocity of 3 μm/s are investigated in real time by X-ray micro–tomography and quantitatively compared with model predictions. Controlled by the wettability of the bead matrix two distinct displacement patterns are found with a transition region of about 30° separating both regimes. Within each regime the displacement behavior is fairly insensitive to the exact contact angle ¹.

A compact front morphology emerges if the invading fluid wets the beads while a fingered morphology is found for non–wetting invading fluids, causing the residual amount of defending fluid to differ by one order of magnitude. The corresponding crossover between these two regimes in terms of the advancing contact angle is governed by an interplay of wettability and pore geometry and can be predicted on the basis of a purely quasi–static consideration of local instabilities that control the local progression of the invading interface as similarly introduced by Cieplack and Robbins for 2D systems ² ³. In particular the absence or the appearance of ‘Burst-Instabilities’ where the local instability occurs when the pressure in a throat exceeds the required filling pressure can be used to distinguish the transition between both wetting regimes. For the non-wetting system where the local front progression occurs mainly by ‘Burst-Instabilities’ an interconnected and very extended network of invading and defending phase develops at later times. The interconnected network of the defending phase is slowly drained by gutter flow leading to an increased residual saturation which is reached only after a substantial flush of the invading phase. If time allows, also the situation of bead and grain packs consisting of heterogeneous bead sizes, grain shapes or heterogeneous wettability will be discussed in brief.
Posters

The Study of Solid Phase Particles Blocking Process based on CT scanning technology

Zhenglan LiNone ; Yonggang DuanNone ; Quantang FangNone ; Mingqiang WeiNone

Corresponding Author(s): 360526227@qq.com

The pore blocking caused by solid particles migration is the major reason to formation damage. In order to further describe the solid particles blocking process, the realistic pore network model is established based on the results of micro-CT scanning. At the same time, the granularity distribution model is generated according to the solid phase particles size distribution. Then the “blocking volume” is introduced to judge whether or not pore blocking happen. Based on the conception of “blocking volume”, pore element is generated and all these characteristic parameters of pore element are calculated such as the flow distribution, pore size, particles granularity, blocking volume. According to the judgement standard, the intrusion ratio of solid particles, the sediment ratio of solid particles, the blocking ratio of solid particles, the sediment depth and the blocking depth are all obtained. In addition to this, the parameter sensitivity analyses of influence factors are taken. Through the study of pore blocking simulation, the aim to predict the probable formation damage caused by solid particles based on the structure of core and particles parameters have been achieved. It provides

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-E / 250

The characteristics of the gas and water flow through the micro-tubes and nanotubes

Author(s): Xiao Hu1

Co-author(s): Fuquan Song 1

1 Zhejiang ocean university

Corresponding Author(s): huxiao0329@163.com

The nanoscale flow characteristics are studied more and more popular recently, especially on the development of shale gas reservoir, and gas transport mechanisms include continuous flow, slip flow, and transition flow, which are complicated problems to study. Herein, experiments on deionized water and gas flow through micro-tubes and nanotubes with diameter of 16μm, 6μm, 124nm and 67nm are carried out to research flow characteristics at nanoscale porous media, respectively.
The experimental results of water flow through microtubes and nanotubes are shown in Figure 1, which shows that the Hagen-Poiseuille equation is valid when the micro-tubes diameter is 16µm, and the experimental flux reduces slightly when the diameter decreases to 6µm. However, the flux of water through nanotubes are even less than the H-P equation by one order of magnitude, and deviations between the experimental flux and the theoretical flux tremendously increase with the decrease of diameters of nanotubes.

Figure 1 Comparison of experimental water flux and Hagen–Poiseuille flux

The experimental results of gas flow through microtubes and nanotubes are shown in Figure 2, which shows that when gas flows through the microtubes with a diameter of 16µm, the experimental flux agrees well with the H–P equation, while the experimental flux slightly increases when the diameter decreases to 6µm. However, the deviations between the experimental flux and the theoretical flux will tremendously increase with the decrease in the diameters of nanotubes from124nm to 67nm. Small nanotube diameters lead to high deviations between the experimental flux and the H–P equation. The flux of the gas flow through the nanotubes is even higher than the H–P equation by one to two orders of magnitude, and the H-P equation considerably underestimates the gas flux at nanoscale.

Figure 2 Comparison of experimental gas flux and Hagen–Poiseuille flux

KEYWORDS: microtubes, nanotubes, shale gas, water, H-P equation

Acknowledgments
This work was supported by the National Natural Science Foundation of China (Grant No 11472246)

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-G / 263

The dynamics of fluid deformation in Darcy scale porous media and impact on mixing

Author(s): Marco Dentz

Co-author(s): Aditya Bandopadhyay ; Daniel Lester ; Tanguy Le Borgne ; Felipe de Barros

1 IDAEA-CSIC
2 IIT Kharagpur
3 RMIT University Melbourne
4 University of Rennes
5 University of Southern California

Corresponding Author(s): marco.dentz@csic.es

Stretching and compression of fluid elements is key for the understanding and quantification mixing and reaction in heterogeneous porous media. We quantify the evolution of the deformation tensor in 2 and 3 dimensional Darcy-scale porous media flows using streamline coordinates. Thus, we derive a stochastic process for the stretching of a material strip in terms of a coupled continuous time random walk which is parameterized by the statistical medium and flow properties. The derived model is compared to direct numerical simulation of flow, particle motion and Lagrangian deformation. The impact on mixing is studied for the evolution of a diffusive material blob in heterogeneous Darcy scale flow.

References:

Acceptance of Terms and Conditions:
Parallel 5-A / 597

The effect of pore scale disorder on unstable multiphase flow at the pore scale.

Amir Riaz

Corresponding Author(s): ariaz@umd.edu

The flow of multiple immiscible fluids at the pore scale is sensitive to local porosity fluctuations that can be measured as pore scale disorder. Our high fidelity direct numerical simulations of pore scale multiphase flow indicate that the degree of disorder governs the expression of viscous instability at the pore scale. Instability is suppressed when porosity is highly ordered even for large viscosity contrasts. While instability appears for even minute deviations away from the ordered state, it saturates beyond a certain threshold that depends on the viscosity ratio. The importance of the length scale of flow paths associated with such behaviors will be reported. Implications for permeability measurement and the construction of REV scale under time varying flow will also be examined.

References:

Poster 2 / 468

The gas mass transport model considering the dynamic change of micro-fracture width in shale

FANHUI ZENG; FAN PENG

1 Southwest Petroleum University

Corresponding Author(s): 379031074@qq.com

Shale gas reservoirs generally develop micro fractures. During pressure-relief production, the change of micro-fracture width caused by stress-sensitivity is an important factor affecting shale gas transport. Based on the cubic grid model, the slippage flow model, the Knudsen diffusion model and the surface diffusion model, a gas mass transport model considering the dynamic change of shale micro-fracture width is established by using elasto-plastic mechanics and desorption theory of adsorption gas, meanwhile, the molecular simulation results verify the reliability of the model. On this basis, considering the dynamic change of micro-fracture width, the law of shale gas mass transport is studied, and the contribution of different transporting mechanisms to the total gas transport is discussed. The results show that: (1) Considering the change of micro-fracture width caused by stress-sensitivity, the model established in this paper can well reflect these coexisting flows including continuous flow, slippage flow, Knudsen flow and surface diffusion flow. (2) Compared with original transporting capacity of unconsidering the change of micro-fracture width, When the formation pressure is higher than 3.4MPa, the change of micro-fracture width decreases the gas transporting capacity, and the minimum transporting capacity is only 0.45 times of the original transporting capacity, while the formation pressure is less than 3.4MPa, the change of micro-fracture width increases the gas transporting capacity, the maximum transporting capacity is 4.5 times of the original transporting capacity. The gas mass transport is negatively correlated with the compressibility of micro fracture and positive correlation with the Young’s modulus and Poisson’s ratio of the rock. When the formation pressure is less than 4MPa, the gas mass transport is positively correlated with the gas desorption. When the formation pressure is greater than 4MPa, The effect of different gas adsorption on gas mass transport is almost the same. (3) Considering the change of the micro-fracture width, only when the micro-fracture width is smaller than nano-scale and the formation pressure is
relatively low, the surface diffusion can exert a great influence on the gas transport. When the contribution of surface diffusion to total gas transport is small, the contributions of slippage and Knudsen flow respectively to total gas transport show a tendency of "shifting from one another". When the proportion of surface diffusion is larger, with the decrease of contribution of surface diffusion, The contributions of slippage and Knudsen flow respectively to total gas transport will increase together in the first stage and then "shifting from one another" in the second stage.

Key words: shale gas; micro-fracture; dynamic micro-fracture width; gas mass transport; effect laws

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-A / 167

The impact of drainage displacement patterns and Haines jumps on CO2 storage efficiency

Ioannis Zacharoudiou\textsuperscript{1}; Edo Boek\textsuperscript{2}; John Crawshaw\textsuperscript{3}

\textsuperscript{1} Imperial College London
\textsuperscript{2} Queen Mary University of London

Corresponding Author(s): i.zacharoudiou@imperial.ac.uk

Injection of CO2 deep underground into porous rocks, such as saline aquifers, appears to be a promising tool for reducing CO2 emissions and the consequent climate change. During this process CO2 displaces brine from individual pores and the sequence in which this happens determines the efficiency with which the rock is filled with CO2 at the large scale. The aim of this work is to better understand the impact of different flow regimes, during immiscible two-phase flow, on the displacement and storage efficiency of CO2 deep in saline aquifers. Using multi-GPU free energy Lattice Boltzmann simulations we directly solve the hydrodynamic equations of motion on a three dimensional geometry reconstructed from micro-CT images of Ketton limestone and consider fluid flows in a range of capillary numbers Ca and viscosity ratios. We first verify the existence of the three typical fluid displacement patterns, namely viscous fingering, capillary fingering and stable displacement \textsuperscript{1}. We examine how these distinctively different flow regimes can affect the displacement efficiency, defined here as the fraction of the defending wetting fluid that has been displaced from the pore matrix when the injected non-wetting phase reached the outlet of the domain. Continuing the injection beyond this point we establish the maximum displacement efficiency or storage capacity. Our results indicate that the maximum displacement efficiency decreases with decreasing Ca. As capillary fingering becomes the dominant displacement process at low Ca, storage efficiency converges to a limiting value irrespective of the viscosity ratio.

Particular focus is given to the low Ca flow regime, where displacements at the pore scale typically happen by sudden jumps in the position of the interface between brine and CO2, Haines jumps. We demonstrate that the method reproduces the expected features of the jumps, i.e. sharp increase in the non-wetting phase velocity, abrupt drop in the pressure signal and significant fluid rearrangement. We quantify the degree of fluid redistribution associated with these sharp events by identifying each event from the pressure signal. Preliminary results from this analysis suggest that pressure fluctuations and waiting times between the jumps follow an exponential distribution, in agreement with theoretical predictions, while the same also applies for the event filling volumes probably due to the extensive fluid redistribution. More importantly a significant decrease in storage efficiency is observed, irrespective of the direction of the jump relative to the overall flow direction, contrary to the arguments by Yamabe et al. \textsuperscript{2}. This is due to irreversible fluid rearrangement during Haines jumps that alters the displacement pathways and renders regions of the porous rock inaccessible to the injected non-wetting fluid. This has important implications in the context of geological sequestration of CO2, as Haines jumps become a limiting factor in the storage process.

References:
Parallel 10-A / 179

The impact of horizontal groundwater flow on the dissolution of CO2 in saline aquifers

Author(s): Ravid Rosenzweig
Co-author(s): Avihi Tsinober ; Itamar Michel-Meyer ; Uri Shavit

1 Geological Survey of Israel
2 Technion, IIT

Corresponding Author(s): rravid@gsi.gov.il

The dissolution of supercritical CO2 in aquifer brine is one of the most important trapping mechanisms in CO2 geological storage. As supercritical CO2 is less dense than the ambient groundwater, the injected CO2 is susceptible to leakage in case that the sealing layer is not perfectly impermeable. However, when CO2 is dissolved in water it is not buoyant anymore. In fact, CO2-saturated water is slightly heavier than CO2-free water. This situation where CO2-free water is overlaid by heavier CO2-rich water, leads to a hydrodynamic instability in which fingers of dense CO2-rich water are formed and propagate downwards, causing the CO2-free water to move upwards [1,2]. This convective process accelerates the dissolution rate of CO2 into the aquifer water. The majority of previous studies assumed there is no natural groundwater flow in the aquifer and neglected the associated hydrodynamic dispersion and therefore assumed there is no effect on the dissolution dynamics. However, it was found that in some of the saline aquifers considered for CO2 storage groundwater flow rate, although small, is not zero [3]. A few studies investigated numerically the effect of groundwater flow and dispersion on dissolution dynamics [4,5] but no experimental evidence was provided yet.

In this research, we study the effect of groundwater flow on dissolution trapping by performing laboratory experiments and conducting numerical simulations. Experiments were performed in a physical aquifer model using a mixture of methanol and ethylene-glycol (MEG) as a CO2 analog while varying the water horizontal flow rate. Simulations were then carried out to reproduce experimental results. We found that water horizontal flow has a significant effect on the dynamic of the instability and the fingers morphology. As the horizontal flow increases, the number of fingers, their wavenumber and their propagation rate decrease. In high water flow rates, no fingers were developed and the dissolution process was driven by diffusion and dispersion alone. While the classic dissolution behavior, consisting of a diffusive regime followed by a convective regime was clearly observed, the effect of water flow on the dissolution rate did not show a clear picture. When increasing the horizontal flow rate, the convective dissolution flux slightly decreased and then increased. It seems that when horizontal flow rate increases, there is a tradeoff between the decay of instability which suppresses dissolution and the increase in dispersive flux and fresh water inflow which enhances dissolution.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-E / 89

The impacts of shale pore structure characteristic on fluid transport properties by a multi-scale pore network model

Wenhui Song\textsuperscript{1} ; Jun Yao\textsuperscript{1} ; Yang Li\textsuperscript{2} ; Hai Sun\textsuperscript{1} ; Lei Zhang\textsuperscript{1} ; Yongfei Yang\textsuperscript{1}

\textsuperscript{1} China University of Petroleum
\textsuperscript{2} Department of Oilfield Exploration & Development, Sinopec

Corresponding Author(s): song_wen_hui@hotmail.com

The organic and inorganic pores exhibit significant differences in pore sizes and surface chemistries that give rise to complex fluid flow behaviours. It is well known that pore size and pore connectivity directly impacts on macroscopic flow properties of a porous medium. Therefore characterization of strong heterogeneous shales with multiscale pore size is indispensable to accurately assess fluid transport properties. Recent advances in pore-scale imaging technique provide practical pathway to understand shale pore structure but the imaging area and resolution is still not available to capture the entire distribution of organic and inorganic pores in a single 2D or 3D image. However, the inorganic pores structure can be accurately captured inthat the inorganic pores sizes are relatively larger. In this work, a multi-scale pore network model is proposed to estimate the fluid transport properties. A 3D binary image is constructed from a section of SEM image which only image inorganic pores. Then the maximal ball fitting method is applied to extract its inorganic pore network. Gas flow inside the nano-porous organic matter considers gas adsorption/desorption, surface diffusion, Knudsen diffusion, viscous flow. Gas flow inside the inorganic pore considers Knudsen diffusion and viscous flow. The constructed multiscale pore network accounts for the distribution of organic matter, organic matter total volume, organic pore size, inorganic pore structure all together. Key analysis results indicate that the distribution of nano-porous organic matter significantly influences the fluid flow ability. Furthermore, the predicted permeability based on the proposed multi-scale pore network model matches well with laboratory measured pressure pulse data.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-H / 319

The importance of inertial effects and Haines jumps in pore scale modelling of drainage displacement for geological CO\textsubscript{2} sequestration
IOANNIS ZACHAROUDIOU, Edo Boek, John Crawshaw

1 Imperial College London
2 Queen Mary University of London

Corresponding Author(s): e.boek@qmul.ac.uk

We investigate pore scale drainage associated with immiscible displacement of brine by CO$_2$ in a porous medium, using state-of-the-art multi-GPU lattice Boltzmann (LB) simulations. Our goal is to better understand the pore scale processes involved in the geological sequestration of CO$_2$. Correctly resolving the pore scale dynamics of multiphase flow in permeable media is of paramount importance for upscaling to reservoir scale displacement processes and the design of efficient CO$_2$ storage operations. Our current investigations are based on previous work on pore-filling events in single junction micro-models and capillary filling mechanisms including Haines jump dynamics. According to the seminal work by Lenormand et al., immiscible displacement can be characterized by only two dimensionless numbers, namely the capillary number $Ca$ and the viscosity ratio $M$, which quantify the ratio of the relevant forces, i.e. the viscous and capillary forces. The above description is thought to be valid in the limit of low Reynolds numbers $Re \to 0$. However, our current investigations reveal that inertial effects cannot be neglected in the range of typical Capillary numbers ($Ca$) associated with multiphase flow in permeable media ($Ca < 10^{-3}$), and accessible to numerical pore scale modeling ($Ca > 10^{-5}$). We observe that, even as $Ca$ and $Re$ decrease, inertial effects are still important over a transient amount of time during abrupt jump events (Haines jumps), when the non-wetting phase passes from a narrow restriction to a wider pore body. Therefore, the description based on the phase diagram of Lenormand et al. may not be sufficient. We include inertial effects by introducing the Ohnesorge number, defined as $Oh^2 = Ca/Re$. We show that this dimensionless number is essential to restrict the parameter selection process, as it is fixed for a given system and independent of the flow rate. We show that the Ohnesorge number reflects the true thermophysical properties of the system under investigation. Considering that the Ohnesorge number is typically in the range of $10^{-5} - 10^{-2}$ for a system of brine-CO$_2$ at the pore scale, it becomes clear that the usual approach in numerical simulations of keeping both $Ca$ and $Re$ low, without respecting the ratio of the two, is fundamentally wrong. Given that inertial effects cannot be neglected in this range of dimensionless numbers, a full Navier-Stokes solver should be used instead of just a Stokes solver, and the value of the ratio $Ca/Re$ should be matched. This approach will resolve the pore scale fluid dynamics correctly. Our results demonstrate that the displacement sequence as well as the fluid distribution in the porous rock can be affected significantly by the choice of the simulation parameters.

References:
2 Ioannis Zacharoudiou, Edo S. Boek, 2016 “Capillary filling and Haines jump dynamics using free energy Lattice Boltzmann simulations”, Advances in Water Resources 92, 43-56

Click here to agree

Parallel 4-G / 678

The influence of Capillary Trapping on Dynamic CO2 Storage Capacity and Long Term Storage Integrity

Author(s): Muhammad Zulqarnain

Page 489
Co-author(s): Mehdi Zeidouni ¹ ; Richard Hughes ²

¹ Louisiana State University
² Craft & Hawkins Department of Petroleum Engineering, Louisiana State University

Corresponding Author(s): mzulpa1@lsu.edu

Containment of injected CO2 is of prime importance for long term integrity of CO2 geological storage projects. Structural/stratigraphic, dissolution, residual, capillary and mineral trapping mechanisms play significant roles on different time scales to keep the injected CO2 within the storage zone boundaries. In heterogeneous media the impact of capillary trapping mechanism becomes significant. Overlooking the capillary trapping contribution may result in underestimating the dynamic storage capacity, and overestimating the leakage risk. In this study the significance of capillary trapping mechanism for a heterogeneous storage zone is highlighted. Publically available well log and petrophysical data is used to construct a representative model of a 1,000 ft thick storage zone in Louisiana, USA. This zone has significant locally interbedded sand and shale intervals that are not continuous over the entire areal extent of the zone. Reservoir simulation is used to model different injection scenarios and resultant movement of CO2 plume. The CO2 is injected for a period of 50 years and then monitored for additional 50 years for its plume movement. In order to capture the contribution of capillary trapping, the capillary pressure for each grid block is scaled by its porosity and permeability values. Therefore each grid block have its own capillary pressure curve, in comparison to a case in which a single capillary pressure curve is used for the entire storage zone. Sensitivity analysis shows that the upward movement of buoyant CO2 plume is substantially impeded by the capillary forces when separate capillary pressure curve is used for each grid block that honors the permeability and porosity of respective block. This results in significant local capillary trapping. This phenomenon has significant implications for dynamic storage capacity and long term stability of CO2 plume. For the studied case, it is observed that capillary trapping mechanism results in enhancing the dynamic storage capacity by a factor of nearly 1.5. It is also observed that the capillary trapping also effects the lateral movement of CO2 plume and CO2 is contained in the storage zone more effectively. The results strongly suggests that for heterogeneous storage zones, ignoring the capillary trapping mechanism can result in significant errors in determining dynamic storage capacity and long term storage integrity.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 978

The transport behavior of the hydraulic fracturing fluid in organic-rich nanoporous shale: A generalized lattice Boltzmann method

Tao Zhang ¹ ; Juntai Shi ² ; Xiangfang Li ³

¹ China University of Petroleum
² China University of Petroleum (Beijing)
³ China University of Petroleum (Beijing)

Corresponding Author(s): tobiascheuing@163.com

During the development of shale gas reservoir, large amount of hydraulic fracturing fluid are forcibly injected into the reservoir to create complex fracture networks. However, field data indicate that only a small fraction of the injected fluid can be recovered during the clean-up period. Except the mostly discussed reasons including capillary force, osmotic-force, and clay hydration, the liquid (fracturing fluid) slip effect in the nanopores of shale matrix might be responsible for this phenomenon as well.
Firstly, the apparent liquid permeability (ALP) model in a single nanopore is established on the basis
of Wu’s model (Wettability effect on nanoconfined water flow, PNAS, 2017), and the model considers the wettability and pore size related liquid slip effect. Then, the model is incorporated into the global lattice Boltzmann method (GLBM) to be scaled up into nanoporous shale. Next, we validated the proposed model by simulating liquid flow in a classical case. Finally, the proposed GLBM is employed to simulate three cases including fracturing fluid flow in a homogeneous shale matrix, a reconstructed shale matrix based on a real SEM image, and a shale matrix in presence of micro-fractures to understand the transport behavior of the fluid in nanopores dominated shale matrix. The flow capability of fracturing fluid in the organic/hydrophobic nanopores of shale matrix is significantly improved due to the huge wall-fluid effect, especially when the radius of the pore is smaller than 100 nm and the contact angle is higher than 120 degrees. After considering the slip effect, the flow field (magnitudes and preferred pathway) of the shale matrix can be significantly changed, and the velocity magnitudes of the region occupied by the organic matter (OM) can even exceed that of the inorganic matter (IOM), although the pores size in the OM is universally smaller than that in the IOM. When the shale matrix contains micro-fractures, the liquid slip effect still has a great impact on the flow enhancement, contributing a lot for the huge fracturing fluid loss in the field. The transport behavior of fracturing fluid in nanopores dominated shale matrix is revealed, and the results implicit that, especially in the organic-rich shale gas reservoir, the fracturing fluid can be infiltrated into the ultra-tight shale formation easier than commonly expected during the hydraulic fracturing operation. This work demonstrates a new insight into the problem of huge fluid-loss reported from the field, providing a theoretical support for development of gas-shale reservoirs.

References:


Acceptance of Terms and Conditions:

Click here to agree

Poster 3 / 993

The wettability of organic rich shales and its effect on transport properties in fractures as realized with the Lattice Boltzmann method
Author(s): Eric Guiltnan

Co-author(s): D. Nicolas Espinoza; M. Bayani Cardenas

1 University of Texas at Austin

2 The University of Texas at Austin

Corresponding Author(s): eric.guiltnan@utexas.edu

The geologic sequestration of CO2 is a potential solution for decreasing anthropogenic atmospheric CO2 emissions by trapping it underground. A primary mechanism for storage is structural trapping where low permeability and high capillary entry pressure caprock materials hold back the buoyant CO2 from rising to the surface. The wettability (or contact angle) of reservoir and caprock materials in relation to CO2 and formation brine partly determines the efficiency of structural trapping. Current practice applies the results of individual reservoir-comprising minerals recorded under laboratory conditions, to rocks under in-situ reservoir conditions. However, the wide variety of measured contact angles reported in the literature calls this practice into question. Moreover, organic shales have not been the focus of systematic studies. Here we analyzed the wettability of CO2 at reservoir conditions on organic shales (Barnett Shale) at various organic matter concentrations and thermal maturities. We found that bulk organic shale remains highly water wet with respect to CO2 despite changes to the maturity or concentration of organics. This finding is in contrast to recent molecular dynamic simulations and our initial expectations from previous pore-scale analyses in which organic matter was shown to be hydrophobic. The results are likely due to the remaining mineralogy of the rock dominating the wetting behavior despite concentrations of organics up to 7.9%. Due to the high porosity of organic matter in shales these bulk, or effective, contact angles may not adequately characterize the wettability of the pore network. To explore this idea further, Lattice Boltzmann simulations on shale fractures with heterogeneous wetting characteristics are presented. The effect of organic matter connectivity on transport properties such as percolation threshold and permeability are explored.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-E / 303

Theoretical foundation of fracture permeability to analyse the flow in channel fracturing based on Navier-Stokes equation

Guoqing XU; Xiaohan Pei; Xianyou Yang; Yang Shi; Yun Jiang; Meng Wang

1 Research Institute of Petroleum Exploration and Development(RIPED), PetroChina,

2 Research Institute of Petroleum Exploration and Development(RIPED), PetroChina

3 Research Institute of Petroleum Exploration & Development, PetroChina

Corresponding Author(s): xgqcup1001@126.com

Channel fracturing, as a novel technology, has received increasing attention in recent years due to its great advantage in promoting the fracture conductivity as well as reducing consumption of water and proppant. The open channels created by heterogeneous distribution of proppant are the priority path for oil or gas to pass instead of the pores exist in proppant pack. Since the flow pattern has been changed from Darcy flow to the flow mode dominated by Navier-stokes percolation by this technique, traditional method to calculate and predict its permeability may not that accurate and appropriate. So this full paper presents a new model to measure the flow capacity of channel fracturing combined with a power law embedment model. The new approach is based on Navier-Stokes equation instead of Darcy-law to compute fracture permeability in channel fracturing. Besides, four influencing, namely, fracture height, proppant pillar size, proppant area friction and embedment, are investigated to analyse their effect on permeability. The proposed analytical model is found to in good agreement with the experimental data, which verifies the precision and the feasibility of this
model. Based on this model, this paper can provide a theoretical basis for channel fracturing design to evaluate the key factor governing the conductivity (permeability), which is helpful to providing a reference for proper pulse time and pumping rate optimization.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 529

Theory and Molecular Simulation of Methane Hydrate in Porous Media

Author(s): Dongliang Jin

Co-author(s): Benoit Coasne

CNRS and Laboratoire Interdisciplinaire de Physique (LIPHY), Universite Grenoble Alpes, F-38000 Grenoble, France

CNRS/University Grenoble Alpes

Corresponding Author(s): dongliang.jin@univ-grenoble-alpes.fr

Methane hydrate is a non-stoichiometric crystalline structure in which water molecules form hydrogen-bonded cages with methane molecules inside. Abundant methane hydrate resources are present on Earth, especially in various mineral porous media (e.g., permafrost and sea-floor). Methane hydrate is important for many applications in the field of energy and environmental science. [2,3] Understanding the formation, stability, and thermodynamics of methane hydrate in porous media has therefore attracted a great deal of attention in the last decade.

The goal of the present work is to combine computer modeling and theoretical approaches to predict the liquid–hydrate–vapor (L–H–V) phase coexistence of methane hydrate confined in porous media. First, molecular simulation, including molecular dynamics, Monte Carlo simulations, and free energy calculations using the Einstein Molecule approach, is used to determine the chemical potential, free energy, and pressure–temperature (P–T) phase diagram for bulk methane hydrate (in equilibrium with liquid water and methane vapor). This strategy also provides a mean to determine the corresponding equilibrium methane occupancy, i.e., the methane composition in the hydrate phase. Then, molecular simulation using the direct coexistence method (DCM) is used to determine the pore size effect on melting temperature $T_m$ of methane hydrate. To do so, methane hydrate and liquid water are confined in porous media with various pore size $D_p$. For each $T$ and $P$, the system is set in equilibrium with an infinite reservoir of particles imposing its chemical potential for each species $\mu_m$ and $\mu_w$ (grand canonical ensemble). At a given $P$, the high symmetry phase (hydrate) will be stable below the melting temperature $T_m$ while the low symmetry phase (liquid) will be stable above $T_m$. Our first results suggest that the shift in melting temperature with respect to the bulk, $\Delta T_m = T_{m,\text{pore}} - T_{m,\text{bulk}}$, is negative. This is consistent with the Gibbs-Thompson equation with a lower hydrate-wall surface tension than the liquid-wall surface tension, which predicts that $\Delta T/T \sim 1/D_p$. A theoretical derivative for such Gibbs-Thompson equation is analyzed, and free energy calculations using umbrella sampling are used to confirm these findings.

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 368
Thermal Analytical Solution for Rate Transient Analysis

Yilin Mao†; Mehdi Zeidouni†

† Louisiana State University

Corresponding Author(s): ymao6@lsu.edu

Pressure-induced temperature transient analysis has emerged recently with the downhole temperature monitoring techniques to characterize the reservoir. In this work, we develop analytical approaches and solutions to model the temperature signals associated with variable rate production of slightly compressible fluid and apply it to several field temperature measurements to characterize the reservoir. The analytical solution presented in this paper is more applicable for field application compared to previous temperature transient analytical solutions assuming constant rate production. This model is derived from the single phase energy balance equation coupled with transient rate and pressure behaviors. Applying the temperature transient analytical solution under boundary dominated flow, the effect of rate variability on temperature signals is well understood and analyzed with the temperature profiles. Various super-position and material balance time procedures are applied for different production scenarios. Simple procedures to apply this model are provided, which present a convenient way to predict the temperature profile. In addition, we provide thermal inversion procedures to characterize the reservoir by evaluating its permeability, porosity, drainage area, and reservoir shape.

The temperature profiles obtained from the analytical solution shows good agreement with those from numerical simulation and are sensitive to total compressibility and reservoir permeability, thickness, and boundary. Sensitivity analyses of temperature profiles are performed on reservoir thickness, permeability, outer boundary radius, total compressibility, fluid specific gravity, specific heat, and viscosity. The early time temperature profiles are induced by pressure transient and followed by the late time effect of boundary dominated flow. With adequate knowledge of other reservoir properties, detailed procedures are demonstrated and can lead to the interpretations of permeability, reservoir boundary, and damaged zone permeability. Even with no prior knowledge of other reservoir properties, simplified procedures reveal several groups of properties. Several field temperature measurements are applied with the developed solution to estimate reservoir properties. The estimations are compared with available properties acquired from other methods to explore the practical purpose of this model. The analytical solution presented in this paper is more applicable for unconventional reservoir characterization application compared to previous analytical solutions for temperature transient analysis.

References:

Mao, Y. 2014. An analytical pressure model to guide downhole sensor placement for carbon dioxide sequestration monitoring. Master of Science, Missouri University of Science and Technology.


Acceptance of Terms and Conditions:

Click here to agree

Parallel 7-B / 7
Thermal conductivity predictions for porous materials via effective medium approximations and cross-property relations

Willi Pabst¹ ; Eva Gregorová² ; Tereza Uhlířová³

¹ University of Chemistry and Technology, Prague
² University of Chemistry and Technology, Prague

Corresponding Author(s): eva.gregorova@vscht.cz

The effective thermal conductivity of porous materials is determined by all details of their microstructure. Since lower bounds (both Wiener and Hashin-Shtrikman bounds) are not available for porous materials (with vacuous voids), all predictions based on the porosity alone are necessarily model-based and thus tentative. In this contribution we first recall the exact solution of the single-inclusion problem for spherical and spheroidal pores ¹, give a comprehensive summary of admissible nonlinear model relations (Maxwell-Èucken relation, Coble-Kingery relation, power-law relation, our exponential relation)² and explicitly exclude those model relations that are either redundant (self-consistent / Landauer-Bruggemann model), non-admissible (Spriggs’ exponential relation) or useless (minimum solid area models)³. Further it is shown how the exact solution for spheroidal pores (oblate or prolate) is to be implemented into the admissible nonlinear effective medium approximations ⁴. In the second part of this contribution we show that the problem of characterizing microstructural details and implementing microstructural information beyond volume fractions can be circumvented via cross-property relations (CPRs). In particular, the knowledge of the relative tensile modulus (Young’s modulus) can be used to predict the relative thermal conductivity of porous materials. The CPRs currently available for this purpose are recalled, including the Sevostianov-Kováčik-Simančík CFR ⁵, our CFR for isometric pores ⁶ and the recently proposed generalized version of the latter for anisometric pores (spheroidal-prolate and spheroidal-oblate) ⁷. Using numerical modeling on a wide range of different computer-generated digital microstructures (convex pores, concave pores, spheroidal pores, foams) it is shown that our CFR provide the best thermal conductivity predictions currently available.

References:


Acceptance of Terms and Conditions:

Click here to agree

Parallel 8-F / 906

Thermo-Chemo-Hydro-Geomechanical Model and Numerical Solution Strategy for Marine Gas Hydrate Geosystems with a focus on Gas Production and related Geohazards
Author(s): Shubhangi Gupta
Co-author(s): Matthias Haeckel; Christian Deunser

1 GEOMAR Helmholtz Center for Ocean Research Kiel

Corresponding Author(s): sgupta@geomar.de

Gas hydrates are crystalline solids formed when water molecules form a cage-like structure and trap a large number of gas molecules within. Gas hydrates are thermodynamically stable under conditions of low temperature and high pressure and occur in nature typically in permafrost regions and marine off-shores. If warmed or depressurized, hydrates destabilize and dissociate into water and gas.

It is widely believed that the energy content of methane occurring in the form of hydrates possibly exceeds the combined energy content of all other conventional fossil fuels put together. Natural gas hydrates are, therefore, deemed a promising future energy resource, and it is of high interest to develop technically and economically feasible methods for producing methane gas from these reservoirs. Several methods have been proposed, such as, thermal stimulation and depressurization. However, there are serious safety concerns regarding the inherent environmental and geotechnical risks associated with gas hydrate destabilization. When the gas hydrates form in natural sediments, they enhance the strength of the sediment and prevent normal consolidation. During gas production, loss of hydrates can cause rapid consolidation, uncontrolled sand migration, bore-hole instabilities and well collapse. Loss in the structural integrity of the sediment around the production well can seriously impact local and regional slope stability. Due to these process management and safety concerns, and large uncertainties associated with the properties, distributions, and hydrogeomechanical behavior of hydrate-soil fabrics, none of the proposed methods have reached the technical maturity which is necessary for large scale gas production, despite a considerable research effort in the past decades.

To make realistic assessments of the viability of any future technology for natural gas hydrate reservoirs, it is important to develop mathematical models and numerical tools that can handle highly coupled multi-physics processes in complex geological settings, and reliably quantify the uncertainties in their predictions for the relevant production scenarios.

Here, we present our modeling and coupling concept for marine gas hydrate geosystems with a focus on gas production and geotechnical risks quantification. In this context, we describe natural gas hydrate reservoirs as highly complex geological porous medium characterized by large material heterogeneities, local anisotropies, and a large number of strongly coupled multi-physics processes, including: 1) kinetically driven hydrate phase change; 2) multi-phase, multi-component fluid flows; 3) thermal effects; 4) geomechanical deformation of the sediment. Central to our coupling concept is the assumption that hydrate and soil form a single composite phase, where, soil forms the primary load bearing skeleton, while the hydrate acts as a mechanical cementing agent which only enhances the strength and stiffness of the composite solid without bearing any load itself. An important consequence of this assumption is that it allows us to define two porosities: One that evolves as a result of sediment deformation, and the other that evolves due to hydrate phase change, thereby, greatly simplifying the mathematical model.

In this presentation, we will describe our mathematical model and numerical solution strategy, and show the applicability of our model through numerical simulation of high pressure flow-through tri-axial experiments.

References:

Acceptance of Terms and Conditions:

Click here to agree

Invited 2 (Room D) - Kamaljit Singh / 1115
Three-dimensional image processing and analysis: segmentation, contact angle and curvature mapping

Kamaljit Singh

1 Department of Earth Science and Engineering, Imperial College London, London, UK

Corresponding Author(s): kamaljit.singh@imperial.ac.uk

Recent advances in three-dimensional imaging, using X-ray micro-tomography (µCT), has allowed to observe fluid configurations in porous media and measure various pore-scale properties such as contact angle, curvature, fluid connectivity (1-6). In general, gray-scale images obtained from µCT are pre-processed to remove artefacts before reconstruction and then filtered to enhance signal-to-noise ratio. Typically, the filtered images are segmented into various phases using a watershed algorithm. However, with recent developments in machine learning algorithms (7), gray-scale images can be effectively segmented without applying a noise-reduction filter, which can produce more accurate segmentation without the risk of possible smoothening of the image (8). This is essential to compute various porous media properties.

The segmented images are traditionally used to characterize the geometry of the pore space and to construct a pore-network representation of it. Most recently, these images have been used to determine the in-situ wettability state of porous media by measuring effective contact angle at the three-phase contact line, either manually (2) or most recently automatically (1, 9). Furthermore, the segmented data can be processed to estimate fluid-fluid curvature (4, 6, 10), which can then be used to calculate capillary pressure using the Young-Laplace equation. Estimation of these pore-scale properties, along with our ability to image dynamic processes using fast synchrotron imaging (3, 11), provide a valuable tool to understand immiscible fluid displacement in porous media, which was mainly restricted to two-dimensional visualization in the past. Although most of the individual three-dimensional image processing methods have already been demonstrated in recent years, the novelty is to integrate them together for the interpretation of µCT fluid flow experiments towards a specific goal.

Apart from the above discussed advances in measuring pore-scale properties, in this talk, I will show some simple tools using an open-access ImageJ software to process tomographic data. Moreover, I will provide examples of image processing that has helped to understand biological systems, particularly, termite nests.

References:


Acceptance of Terms and Conditions:

Click here to agree
Parallel 1-D / 809

Tomographic PIV of low to high Re flow through well-ordered porous media

Sofia Larsson¹ ; Staffan Lundström² ; Henrik Lycksam³

¹ Fluid mechanics, Luleå University of Technology
² Fluid Mechanics, Luleå University of Technology, Sweden
³ luid Mechanics, Luleå University of Technology, Sweden

Corresponding Author(s): sofia.larsson@ltu.se

Pressure-driven flow within the plane of a confined thin porous medium takes place in a number of natural and industrial processes. This includes flow during manufacturing of fibre reinforced polymer composites with liquid moulding processes, passive mixing in microfluidic systems and paper making. The thin porous media considered here is a simplified, well-structured model of a porous media where the solid parts have the shape of vertical cylinders placed on equal interspatial distance from each other in a quadratic pattern. The array of cylinders are confined between two parallel plates, hence the permeability depends on both the diameter and height of the cylinders, as well as their interspatial distance. In order to study the flow tomographic Particle Image Velocimetry is used and the fluid is indexed matched so that a whole volume of the flow can be scrutinized without optical distortion in each measurement. The results reveal that the averaged flow field changes substantially and that the wakes formed behind the cylinders plays a major role.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 854

Toward direct pore-scale reactive modelling of low-salinity flooding in 2D/3D porous media images

Julien Maes¹ ; Sebastian Geiger¹

¹ Heriot-Watt University

Corresponding Author(s): j.maes@hw.ac.uk

We present a two-phase multicomponent reactive pore-scale model based on Direct Numerical Simulation of the Navier-Stokes equations using the Volume-Of-Fluid and the Continuous Species Transfer methods. In order to study wettability change during low-salinity flooding, simple upscaling rules from the nano-scale to the pore-scale are integrated to the model to describe (1) change of local contact angle with change of electrical double layer potential, (2) effect of ionic transport and electrical field in the water thin film and (3) ganglion remobilization due to build-up of osmotic pressure in the thin film. We show that our model can be fitted to match experimental results of oil recovery by low-salinity effect. We then investigate the impact of each mechanism on the increase of oil recovery during low-salinity flooding in 2D/3D porous media images.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 524
Towards a better understanding of foam flow patterns in porous media

Author(s): Christopher Yeates¹
Co-author(s): Souhail Youssef ¹ ; Lahcen Nabzar ¹ ; Guillaume Batot ¹
¹ IFPEN

Corresponding Author(s): christopher.yeates@ifp.fr

Liquid foams are a proposed solution to overcoming conformance issues while increasing apparent viscosity over gas/water only injections in petroleum reservoirs. However due to the diversity of flow behaviour foam flow in porous media providing a sufficiently accurate and low uncertainty model for industrial use can represent a significant challenge. Understanding the specifics of foam flow dynamics in terms of elements of the porous media microstructure could alleviate some of the task involved with describing foam displacements.

In our study we make use of a microfluidic experimental setup including a high speed camera (800 fps obtained in one configuration), and precise fluid injection rates and measured pressure drop over a 2D micromodels of varying structure through which we observe foam flow. A significant increase in viscosity is observed as the pressure drop rises until obtaining a smooth pressure profile interpreted as the steady state. To obtain quantified data regarding foam bubble population and transport, an image processing workflow was developed that involves binarizing the images through a thresholding method based around the foam films, then successively eliminating the objects representing the solid grains impeding flow. The final step of the workflow involves tracking individual bubbles through the image series, and averaging the results over multiple image series. The dynamic tracking of a high number of objects (approx. 5 000 000 velocity data points per model heatmap) allows us to establish of steady state velocity and flux fields within the medium. This data is furthermore combined with the bubble sizes. In this way the flow behaviour can be observed in terms of either flow velocity per bubble size or inversely.

Initial results of velocity and flux fields demonstrate that significant differences exist between flow of differing bubble sizes. Whether it be through self-segregation or bubble size adaptation, the flow of largest bubbles is exclusively found in a few paths that are seen to be on average wider and oriented in parallel to the flow. These paths are also more likely to carry higher velocities. On the contrary, the smallest bubbles populate transverse small pathways perpendicular to the flow direction. For a means of comparison, we perform 2D Lattice Boltzmann simulations of simple Stokes flow on a digitized template of the micromodel, and compare the obtained foam fluxes with the monophasic numerical analogue. When compared to the monophasic flow simulations, the amount of transverse flux in paths perpendicular to the flow direction is much smaller in all the foam examples.

Through a more quantitative analysis flow in terms of microstructural parameters we explore relationships (or lack thereof) between foam flow and local porous media properties such as pore/constriction sizes, coordination and immediate neighbourhood properties. Foam flow is only weakly correlated to pore scale properties as in a steady state situation the entirety of a flow path over the medium has to be taken into account as a single flowing object and flow preference needs to be evaluated in terms of the complete path properties.

References:

Click here to agree

Parallel 5-H / 841
Tracer Transport Characterization of Interactions Between Resident and Infiltrating Water During Drainage-Imbibition Cycles

Brian Berkowitz\textsuperscript{1} ; Pei Li\textsuperscript{None}

\textsuperscript{1} Weizmann Institute of Science

**Corresponding Author(s):** pei.li@weizmann.ac.il

We quantify interactions between resident and infiltrating water coupled with tracer transport during water-air, drainage-imbibition cycles. Using a 2D Lattice Boltzmann method (LBM), we investigate immiscible-miscible and tracer transport processes in an heterogeneous pore structure with various boundary conditions. The simulations clearly show three types of interactions between resident and infiltrating water: (1) flushing of resident water; (2) mixing between resident and infiltrating water; and (3) bypassing of resident water. Some of the (initial) resident water, containing tracer, remains in the pore space, especially larger pores, even after two drainage-imbibition cycles. We analyzed the sensitivity of these three types of interactions to flux on the boundary, contact angle, body force and porosity. The results on ‘old’ and ‘new’ water saturation, pockets number and the tracer concentration in the outflow demonstrate that the boundary flux and the porosity are critical factors affecting these interactions. Thus, the initial saturation and distribution of resident water are not the only factors affecting interactions between resident and infiltrating water. Although it is difficult to directly link such pore-scale simulations to macroscales, the results show a certain correlation to field-scale phenomena: similar to field measurements, we find that infiltrating water represents the majority of water reaching the domain outlet at short times with higher input flux, while a mixture of resident and infiltrating water then elutes over longer times with lower input flux. Our simulations also show intrinsically how resident water can remain in the domain over long times (months and even years), as found at the field scale, and demonstrate that LBM is capable of simulating transport phenomena in partially saturated porous media.

References:

**Acceptance of Terms and Conditions:**
Click here to agree

---

**Transport of Bitumen as Water-External Emulsion in Porous Media**

Kai Sheng\textsuperscript{1} ; Francisco Argüelles-Vivas\textsuperscript{1} ; Kwang Hoon Baek\textsuperscript{1} ; Ryosuke Okuno\textsuperscript{1}

\textsuperscript{1} The University of Texas at Austin

**Corresponding Author(s):** ksheng@utexas.edu

Water is the most predominant component in steam injection processes, such as steam-assisted gravity drainage (SAGD). The main hypothesis in this research is that in-situ oil transport can be substantially enhanced by generating oil-in-water emulsion, where the water-continuous phase acts as an effective oil carrier. The objective of this paper is to evaluate the capability of oil-in-water emulsions to transport bitumen in porous media within a temperature range of 350 – 470 K at 3.5 bar. Athabasca bitumen and two organic alkalis of different chemical structures were used in this research. An alkali concentration of 0.5 wt% was found optimal to form oil-in-water emulsions with bitumen and NaCl brine at a range of salinity. In-line density measurements were conducted to confirm that there was single-phase emulsion in a 200-ml accumulator. Then, flow experiments through glass beads packs were carried out to estimate effective viscosities of oil-in-water emulsions at typical shear rates in oil sands under SAGD (e.g., 1 to 10 [1/sec]). The bitumen concentration in each emulsion sample was quantified directly by using an emulsion breaker. Finally, emulsion molar flow rates were calculated with an analytical equation of gravity drainage.
Emulsion viscosity measurements showed shear-thinning behavior with much lower viscosity than the original bitumen. At an estimated shear rate of 1.0 per second, for example, the viscosity of oil-in-water emulsion for 0.5 wt% alkali was 12 cp at 350 K, which is much lower than the original bitumen viscosity, 190 cp, at the same temperature.

The obtained experimental data, such as effective emulsion viscosity, bitumen content in emulsion, and properties of the porous media used, were then used to quantify the bitumen molar flow under gravity drainage. Results showed that oil-in-water emulsion can enhance in-situ bitumen transport by a factor of 4 in comparison with SAGD, and by a factor of 2 in comparison with hexane-SAGD.

This research demonstrate that the clear advantage of bitumen transport via water-external emulsion can be obtained by adding only 0.5 wt% of alkali in brine. The mobility of the bitumen-containing phase is substantially enhanced because the oil-in-water emulsion flows as a single phase with a much lower viscosity. In contrast, conventional solvents, such as n-alkane mixtures, reduce bitumen viscosity by dilution using a substantial amount of those expensive solvents.

A difference between the two alkalis used is in their ability to dissociate in water; one of the alkalis has three more dissociation sites than the other. This led to different phase behaviors and rheological properties observed in our experiments.

This is the first time the potential of organic alkalis to improve bitumen transport is quantified experimentally. The experiments were newly designed to evaluate the molar flow rate of oil-in-water emulsions at SAGD operating conditions. The alkaline concentration required for effective bitumen transport is even lower than 1 wt% in the brine. Recovery mechanisms of alkali-SAGD are explained in detail, and compared to the flow characteristics in SAGD and other solvent-assisted SAGD.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-F / 291

Transport of deformable polymer particle gels in heterogeneous porous media by IB-LBM simulation

Author(s): Wenhai Lei

Co-author(s): Chiyu Xie ; Moran Wang

Corresponding Author(s): leiwh16@mails.tsinghua.edu.cn

Non-uniform fluid displacements in heterogeneous porous media are commonly observed, while are unfavorable in oil/gas recovery processes. Recently, the deformable polymer particle gels such as preformed particle gel (PPG) and soft micro-gel (SMG) were successfully applied to improve the sweep efficiency under such bad conditions. Although experimental studies presented qualitative observations of their in-depth plugging and flowing diversion capabilities, deeper numerical mechanisms on the deformable polymer micro-gels for enhanced oil recovery (EOR) are still rare. The difficulties mainly lie in the following reasons: (1) the migration of deformable polymer particle gels is non-continuous, invaliding the classical continuum based theories; (2) viscoelastic behaviors of the gel particles should be considered and (3) the problem is confined in the complex porous geometries.

In this paper, an Immersed Boundary-Lattice Boltzmann (IB-LBM) framework is established to capture the motion of viscoelastic polymer micro-gels in porous media. The LB method is used to solve the Navier-Stokes equations in a Eulerian coordinate for the main flow field. The fluid–particle interaction is carried out by coupling with the IB scheme within a Lagrangian coordinate. The viscoelastic deformation and behaviors of the particles are recovered by the capsule model containing a spring-network model and by setting another kind of fluid property. Primarily, the critical size of a polymer particle gel to deform and pass through one single throat is
studied. We find that the different geometry (particle-throat diameter ratio, the length of the throat), pressure gradient and the viscosity ratio are key factors. Thence we investigated the transport of the polymer micro-gels in the cross-shaped channel with heterogeneity. Once the gel is placed in the higher permeable zone, the resistance in this zone will increase. Thus the following injected water will be diverted into the lower permeable zone and help the residual oil displacement there. Our results improve the understandings of the mechanisms of the deformable polymer particle gel for enhancing oil recovery in heterogeneous porous media.

References:

Click here to agree

Poster 3 / 846

Transport of polymer particles in an oil-water flow in porous medium: enhancing oil recovery

Max Endo Kokubun¹; Florin Radu¹; Eirik Keilegavlen¹; Kundan Kumar¹; Kristine Spildo¹

¹ University of Bergen

Corresponding Author(s): max.akira@gmail.com

We study a simple model for the transport of polymer particles injected along with water in a porous rock containing oil. The main goal of this technique is to recover oil that remains trapped after waterflood. Such enhancement occurs through a microscopic diversion of the water flow caused by clogging of narrow pore throats by the injected particles. The diverted flow may lead to the mobilization of oil which was initially trapped. Experimental results indicate that heterogeneous cores are more favorable to accumulation of particles in pore throats. Moreover, that the accumulation of particles is a dynamic process: unclogging may occur as well. We propose a simple model which accounts for the transport of polymer particles and accumulation and release of them at pore throats. We show that a non-equilibrium reaction model can reproduce qualitatively the experimental results.

References:
K. Spildo, A. Skauge, M.G. Aarra, M.T. Tweheyo
A new polymer application for North Sea reservoirs
SPE 113460 (2009)
T. Skauge, S. Hetland, K. Spildo, A. Skauge
Nano-sized particles for EOR
SPE 129933 (2010)
C. Gruesbeck, R.E. Collins
Entrainment and deposition of fine particles in porous media
F. Civan
Modified formulations for particle deposition and removal kinetics in saturated porous media

Click here to agree
Parallel 9-B / 125

Transport processes and water based ink – paper interactions

Nicolae Tomozeiu¹

¹ Océ-Technologies B.V.

Corresponding Author(s): nicolae.tomoeziu@oce.com

The inkjet technology fuels the rapidly evolving world of printing. This printing technology delivers
good print quality using the flexibility of digital printing at a breakthrough cost price. The R&D
department of Océ Technologies, a Canon company, is a major player in the development of inkjet
technologies for many different applications.

Liquid spreading, evaporation and imbibition into porous material are physical processes that de-
scribe the interactions of aqueous ink with paper. Understanding them is vital to have prints of high
quality; and this is the aim of this work. The influence of the liquid physical properties as well as
of the paper characteristics will be considered. Experimental studies based on optical spectroscopy,
microscopy, Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR) and Auto-
matic Scanning Absorptometer (ASA) are presented within this work revealing the today level of
understanding the transport of complex liquids into porous media. For each method of investigation
we will present the main models, including their strengths and limitations.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-A / 352

Transport with Bimolecular Reactions in Fracture-Matrix Systems: Analytical Solutions with Applications to Weathering Reactions and In-Situ Chemical Oxidation

Harihar Rajaram¹ ; Masoud Arshadi²

¹ University of Colorado, Boulder
² Tufts University

Corresponding Author(s): arshadi@colorado.edu

We consider the problem of advection, matrix-diffusion and bimolecular reactions in fracture-matrix
systems, with two example applications: (i) Weathering reactions in fractured bedrock and (ii) in-situ
chemical oxidation (ISCO) for remediation of fractured rock. In both cases, a reagent (a weathering
agent such as H+ or dissolved oxygen, or permanganate in the case of ISCO) are supplied through
a fracture, and react with a second species (immobile mineral species in the case of weathering re-
actions, or TCE/PCE in the case of ISCO) initially contained in the fracture-matrix system. In both
cases, moving reaction fronts form and propagate along the fracture and into the rock matrix. The
propagation of these reaction fronts is strongly influenced by the heterogeneity/discontinuity across
the fracture-matrix interface (advective transport dominates in the fractures, while diffusive trans-
port dominates in the rock matrix). We present analytical solutions for the concentrations of the
oxidant/weathering agent, weathering mineral or TCE and natural organic matter; and the propaga-
tion of the reaction fronts in a fracture-matrix system. Our approximate analytical solutions assume
advection and reaction dominate over diffusion/ dispersion in the fracture and neglect the latter. In
the ISCO problem, the behavior of the reaction-diffusion equations in the rock matrix is posed as a
Stefan problem where the supplied oxidant reacts with both diffusing (TCE) and immobile (natural
organic matter) reductants. Our analytical solutions establish that the reaction fronts propagate dif-
fusively (i.e. as the square root of time) in both the matrix and the fracture. Our analytical solutions
agree very well with numerical simulations for the case of uniform advection in the fracture. In the
context of the ISCO problem, we also present extensions of our analytical solutions to non-uniform flows in the fracture by invoking a travel-time transformation. These non-uniform flow solutions are relevant to field applications of ISCO, which employ forced-gradient flow systems. Our approximate analytical solutions are relevant to a broad class of reactive transport problems in fracture-matrix systems where moving reaction fronts occur, and may be generalized further to consider multiple interacting species.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 542

Tuned Nanoparticle Deposition In Porous Media To Improve Efficiency of Nanoremediation

Carlo Bianco¹ ; Janis Patino³ ; Tiziana Tosco¹ ; Alberto Tiraferrí¹ ; Rajandrea Sethi¹

¹ DIATI, Politecnico di Torino

Corresponding Author(s): tiziana.tosco@polito.it

Nanoremediation is an innovative environmental nanotechnology aimed at reclaiming contaminated aquifers. It consists in the subsurface injection of a reactive colloidal suspension for the in-situ treatment of pollutants. The greatest challenges faced by engineers to advance nanoremediation are the effective delivery and the appropriate dosing of the nanoparticles into the subsoil. These are necessary for the correct emplacement of the in situ reactive zone and to minimize the overall cost of the reclamation and the potential secondary risks associated to the uncontrolled migration of the injected particles.

In this study, a model assisted strategy, called NanoTune, is developed to control the distribution of colloids in porous media. The proposed approach consists in the sequential injection of a stable suspension of reactive nanoparticles and of a destabilizing agent with the aim of creating a reactive zone within a targeted portion of the contaminated aquifer. The controlled and irreversible deposition of the particles is achieved by inducing the mixing of the two fluids in the desired portion of the aquifer.

This approach is here exemplified by the delivery of humic acid-stabilized iron oxide nanoparticles (FeOx), a typical reagent for in situ immobilization of heavy metals. Divalent cations, which are known to cause rapid aggregation of the suspension because of their strong interaction with the humic acid coating, are used as destabilizing agents. The injection strategy is here applied in 1D columns to create a reactive zone for heavy metal removal in the central region of the sandy bed. The software MNMs was used to assess the correct sequence and duration of the injection of the different solutions in the 1D medium. Moreover, the numerical code MNM3D (MNM3D - Micro and Nanoparticle transport Model in 3D geometries) was developed by the authors of this work to support the case-specific design of the injection strategy during field scale applications.

The NanoTune approach represents an advancement in the control of the fate of nanomaterials in the environment, and could enhance nanoremediation making it an effective alternative to more conventional techniques.

Co-funded by: EU H2020 Regrround Grant Agreement No. 641768

References:


Acceptance of Terms and Conditions:
Click here to agree

Poster 4 / 461
Uncertainty Quantification in DFN simulations with random geometry

Stefano Berrone¹ ; Sandra Pieraccini² ; Stefano Scialò² ; Fabio Vicini²

¹ Politecnico di Torino, Italy
² Politecnico di Torino

Corresponding Author(s): stefano.scialo@polito.it

In the framework of underground flow simulations in fractured media, modeled by Discrete Fracture Networks (DFNs), we focus on the issue of the non-deterministic description of the network. For performing numerical simulations, fractures are indeed typically sampled from probabilistic distributions for both hydro-geological properties (fracture transmissivity) and geometrical features (orientation in the 3D space, position, size). An uncertainty quantification analysis is mandatory in these situations, for assessing the impact of stochastic parameters on some relevant quantities of interest (as, for example, the equivalent permeability). In the relevant case of stochastic description of the geometry of the network, the network connectivity may change among samples; as a consequence, the quantity of interest is likely to display a non-smooth behavior in the space of stochastic parameters. This situation is known to represent a challenging issue also for modern UQ techniques such as stochastic collocation strategies. We will address the issue of the application of effective, modern UQ techniques, as the Multilevel Monte Carlo Method (MLMC), for accurately computing suitable statistics of the quantity of interest at a moderate computational cost, considering both stochastic transmissivities and stochastic geometrical parameters.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 10-G / 560

Understanding Wicking in Textile by Multiscale Imaging and Modeling

Author(s): Robert Fischer¹

Co-author(s): Dominique Derome ² ; Jan Carmeliet ³ ; René Rossi ¹

¹ Empa Swiss Federal Laboratories for Materials Science and Technology
² Empa
³ ETH Zurich

Corresponding Author(s): robert.fischer@empa.ch

Textiles are porous media found in a wide variety of configurations, resulting from weaving, knitting or crocheting yarns into networks. Textiles consist of multiple scales of fiber, yarn, fabric and multilayered systems, each showing their own porosity system and complexity. Wicking, or the spontaneous liquid capillary uptake in the resulting multiscale pore system, needs a multiscale approach. We present a multiscale framework to predict the wicking behavior incorporating pore network modeling and continuum transport modeling approaches, using high-resolution lab X-ray tomography for identifying the pore configurations. For validation, we use synchrotron X-ray fast-tomography of water uptake at yarn scale and neutron projection at textile scale. At yarn scale, we first obtain the yarn configuration by highly resolved submicron X-Ray computed tomography. Then, we extract, from this geometry, the information required to develop a pore network capturing all the appropriate complexity, namely long undulating pores, with a loose system of throats and contacts. The configuration of yarns is particularly challenging when analyzed towards building a pore network. Then we develop a pore network model that allows simulating capillary uptake in the yarn system. Given the long aspect ratio of these pores, we track the developing of
liquid film building up along the yarn and filling up of the yarn pore space. We then isolate a representative element of the textile. Knowing the intra-yarn structure and transport properties, we examine the inter-yarn wicking properties by imaging fabric structures at lower spatial resolution of several microns but larger field of view. A mesoscale pore network is constructed on top of the microscale yarn pore network. This modeling approach gives us the three-dimensional permeability tensor of a given fabric element, i.e. a certain knitting stitch or woven pattern. Fabrics are repetitive patterns of such structural elements. We use the derived mesoscale transport properties to model the water transport on fabric scale. A Darcy’s type continuum approach allows us to predict the wicking behavior of different fabric patterns, also considering gravity. Previous neutron projection experiments and finite-element modeling studies showed good agreement of the multi-porous modelling with the observed wicking behavior (Parada et al. 2017a,b).

Understanding the capillary uptake and redistribution of liquid water in textile not only can improve comfort in clothing but also protect firefighters under extreme conditions or find application in medicine.

References

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-D / 724

Understanding the influence of small scale geological heterogeneity on capillary trapping of CO2 using engineered beadpacks

Author(s): Prasanna Krishnamurthy

Co-author(s): Luca Trevisan 2; Timothy Meckel 3; David DiCarlo 1

1 The University of Texas at Austin
2 Karlsruhe Institute of Technology
3 Bureau of Economic Geology, The University of Texas at Austin

Corresponding Author(s): prasannagk@utexas.edu

During geologic CO2 sequestration, most of the storage domain far from the injection sites is likely to be dominated by buoyancy and capillary forces. Under such flow regimes, small scale geological heterogeneities have been shown to dampen plume migration rates and cause trapping beneath capillary barriers. To understand the impact of such heterogeneities on CO2 trapping processes experimentally, many core-scale and lab scale flow studies have been conducted. Reservoir cores are limited by the scale of investigation possible and most lab experiments are conducted in macroheterogeneous media constructed by arranging homogeneous units to represent heterogeneity. However, most natural sedimentary facies display heterogeneity at a hierarchy of scales, and heterogeneity at the mesoscale (mm to decimeters) goes unrepresented in laboratory experiments due to the difficulty in reproducibility.

This work presents results from buoyancy driven migration experiments conducted at the meter scale using glass beads packed in a quasi 2D glass cell and complementary reduced physics simulations. We demonstrate a novel automated technique to build beadpacks with 2D heterogeneous sedimentary features in a reproducible manner. A fluid pair that mimics the phase density and viscosity contrasts, and interfacial tension of CO2-Brine at reservoir pressures and temperatures is employed for the flow experiments. Light transmission technique is used for visualization, and to calibrate and quantify saturation of the trapped non-wetting fluid during the experiments. Invasion Percolation is used to simulate the buoyancy driven flow. With the ability to generate different
types of heterogeneous structures in a reproducible manner, and by comparing experiments and simulations, a systematic investigation of the effect of heterogeneity on capillary trapping becomes possible.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 4-A / 216

Unified presentation and comparison of various formulations of the phase stability and phase equilibrium calculation problems

Tomáš Smejkal\textsuperscript{None} ; Jiří Mikyška\textsuperscript{None}

Corresponding Author(s): smejkto5@fjfi.cvut.cz

We present general formulations of the phase-equilibrium and phase-stability problems for multicomponent mixtures and verify that these formulations generalize the problems of phase-equilibrium and phase-stability at constant volume, temperature, and mole numbers \((VTN\)-flash), at constant internal energy, volume, and mole numbers \((UVN\)-flash), and at constant pressure, temperature, and mole numbers \((PTN\)-flash). Furthermore, we develop a numerical method for solving the general formulation of phase-equilibrium problems. This algorithm is based on the direct minimization of the objective function with respect to the constraints. The algorithm uses a modified Newton-Raphson method, along with a modified Cholesky decomposition of the Hessian matrix to generate a sequence of states with decreasing values of the objective function. The algorithm was implemented in C++ and using generic programming we have a single, portable solver for all three flash formulations. Properties of the algorithm are shown on phase-equilibria problems of multicomponent mixtures in different specifications and with different levels of difficulty. Complexities and numerical performance of the individual flash formulations are discussed.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 963

Universal Scaling Relation for Kinkenberg Flows in Nanoporous Media

Xiangyu Yu\textsuperscript{1} ; Ye Tian\textsuperscript{1} ; Jun Li\textsuperscript{2} ; Xiaolong Yin\textsuperscript{1} ; Keith B. Neeves\textsuperscript{1} ; Yu-Shu Wu\textsuperscript{1}

\textsuperscript{1} Colorado School of Mines
\textsuperscript{2} King Fahd University of Petroleum and Minerals

Corresponding Author(s): xyin@mines.edu

In this study, slip flow of gases were measured in several tight reservoir rock samples and nanofluidic chips. The results were then compared to gas flow simulations by DSBGK. Klinkenberg permeability of rocks was obtained using a steady-state method under varying pore pressures but constant temperature and effective stress. Experiments conducted in nanofluidics devices, which have controlled pore size, also used the steady-state method. Same gas was used in both experiments, making them directly comparable. Independent DSBGK simulations were carried out on several constructed geometry models. The Klinkenberg factors obtained from these independent studies varied across
three orders of magnitude, yet they all collapse on a single scaling relation that indicates that the Klinkenberg factor is inversely proportional to the square root of the intrinsic permeability.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-F / 459

Upscaling Anomalous Gas Behavior in Nanopores in a Multiporosity Shale Gas: Impact on Macroscopic Mass Transfer and Shape Factors

Patricia Pereira¹ ; Aline Rocha² ; Márcio Murad³

¹ Laboratório nacional de Computação Científica (LNCC)
² Laboratório nacional de Computação Científica (LNCC)
³ Laboratório nacional de Computação Científica (LNCC)

Corresponding Author(s): patricia@lncc.br

We consider a shale gas reservoir with multimodal distribution composed of networks of natural and hydraulic fractures along with nano and micropores dispersed within the organic and inorganic matters.

Under the long term pseudo-steady state regime, characterized by the absence of pressure variability in the matrix, mass transfer between matrix and fractures can be approximated by the classical resistance law, which requires the precise evaluation of the shape factor.

Such a framework is well established for bulk fluids in a matrix composed of a single solid phase but still not well understood for highly reactive systems such as shale, characterized by the presence of both organic and inorganic matters.

By proceeding within the framework of formal homogenization, we analyze precisely the influence of gas adsorption in the organic matter and Knudsen effects on the validity of the pseudo-steady regime and the magnitude of the shape factor. By discretizing the coupled non-linear diffusion equations by the Finite Element Method, numerical experiments illustrate the influence of gas adsorption and organic matter upon the accuracy of the pseudo-steady regime for several arrangements of fracture networks.

References:


Acceptance of Terms and Conditions:
Click here to agree

Parallel 6-A / 29
Upscaling of coupled geomechanics, flow, and heat, in a poroelastic medium in the quasi-static situation

Mats Brun¹ ; Florin Radu¹ ; Inga Berre¹ ; Jan Nordbotten¹

¹ University of Bergen

Corresponding Author(s): mats.brun@uib.no

Motivated by geothermal energy storage in the subsurface, we undertake a formal derivation of a linear poro-thermo-elastic system within the quasi-static framework. This derivation is based upon the well known derivation of the quasi-static poroelastic equations (also known as the Biot consolidation model) from the micro structure, except that we now include energy conservation equations in the micro-scale model. These are coupled to the fluid/structure model by using linear thermoelasticity for the solid structure instead of the usual linear elasticity. The resulting upscaled system is similar to the linear poro-elastic equations, but with an added conservation of energy equation, fully coupled to the momentum and mass conservation equations. We start at the pore scale, and apply the technique of homogenization to derive the upscaled model in the case of periodically distributed pores. Assuming the homogenization ansatz holds true, we obtain a fully coupled system of equations on the macro-scale accounting for the effects of geomechanics, heat transfer, and fluid flow within a fully saturated porous material.

References:

Acceptance of Terms and Conditions:
Click here to agree

Poster 2 / 994

Upscaling of mass transfer in field-scale discrete fracture networks using fractional-derivative models

Bingqing Lu¹ ; Yong Zhang¹ ; Donald Reeves² ; HongGuang Sun³ ; Chunmiao Zheng⁴

¹ University of Alabama
² Western Michigan University
³ Hohai University
⁴ Southern University of Science and Technology

Corresponding Author(s): matt.reeves@wmich.edu

Mass transfer in field-scale discrete fracture networks (DFNs) is affected by the erratic internal structure and hydrogeological properties of the fractured media, which can result in non-Darcian flow due to channeling flow and non-Fickian transport due to matrix diffusion competing with fast displacement along fractures. This study explores flow and transport dynamics in various DFNs with a wide range of physical properties using the Monte Carlo simulation approach. The resultant mass transfer dynamics are then quantified by fractional-order derivative models built upon the promising fractional calculus. We will report results implying information transfer from non-Darcian flow to non-Fickian transport, and we will also try to explore the quantitative linkage between these two related processes. The goal is to develop efficient upscaling approaches using the spatiotemporally non-local fractional-derivative equations to characterize mass transfer in field-scale fractured media, without the need to map individual rock fractures.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 6-A / 61

Upscaling of two-phase flow in porous media with free boundary at the pore scale.

Author(s): Sohely Sharmin

Co-author(s): Carina Bringedal ; Sorin Pop

1 Hasselt University

Corresponding Author(s): sohely.sharmin@uhasselt.be

Reactive flows and transport models through the porous medium are important for a wide range of scientific and industrial processes. Examples in this sense are groundwater remediation, oil recovery from reservoirs, CO2 sequestration etc. The main goal of the research is to develop mathematical models that describe such processes at the pore scale and to derive effective models at the macro (Darcy) scale through analytical upscaling. A particular feature of the models addressed here is the occurrence of freely moving interfaces separating different phases, like fluid-fluid (two-phase/unsaturated flow) or solid-fluid (one-phase flow with dissolution/precipitation) at the pore scale. The focus of the research is to give a rational derivation of the upscaled models, which are not only less complex to describe, but also very efficient to simulate. To this aim, homogenization theory based on asymptotic expansion is applied.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-G / 913

Upscaling the Navier-Stokes Equation for Turbulent Flows in Porous Media Using a Volume Averaging Method

Author(s): Brian Wood

Co-author(s): Xiaoliang He ; Sourabh Apte

1 Oregon State University

Corresponding Author(s): brian.wood@oregonstate.edu

Turbulence in porous media is a phenomena that is more prevalent than commonly thought. Such flows happen in packed bed reactors (e.g., oxidation of petrochemicals), in pebble-bed nuclear reactors (where Reynolds numbers can be on the order of 100,000), and at the fluid-solid interface of rivers to name a few examples. One of the characteristics of turbulent flows is the notable deviation from Darcy’s law; the resulting flows are nonlinear, and are described by more-or-less empirical formulations referred to here as the Darcy-Forchheimer-Ergun equation.

In this work, we take a unique approach to the problem by combining conventional volume averaging theory with direct numerical simulation (DNS). Direct numerical simulation seeks to eliminate the closure models conventionally used in turbulence theory with simulations of all relevant time and length scales all the way down to the scale of viscous dissipation. DNS simulations are computationally intensive, requiring potentially millions of degrees of freedom to simulate even simple systems containing a small number of grains. The problem of resolution becomes significantly more difficult as the Reynolds number increases.

For the work we report, we provide (1) a revised examination of the upscaling problem as originally examined by Whitaker (1996), (2) development of a novel closure scheme for relating the microscale velocity deviations to the effective macroscale momentum equation, and (3) the results of a sequence
of high-Reynolds-number flows, with Reynolds numbers up to 1000. Our DNS results validate our proposed closure scheme; comparison of the upscaled and DNS momentum balances show that the predicted macroscale flow parameters are able to reproduce the integrated results of the DNS simulations with high fidelity.

References:
Click here to agree

Parallel 2-H / 703

Urban aquifer hydraulic conductivity estimation and uncertainty analysis

Xin Su\textsuperscript{None}, Valentina Prigiobbe\textsuperscript{None}

Corresponding Author(s): xsw1@stevens.edu

Urbanization in coastal areas has been on an increasing trend during the last century. In some coastal regions, groundwater is one of the major source of potable water for the population, the industry, and the agriculture with an average demand of 30 m3/s \cite{1,2}. Sea-level rise has been recorded to be approximately 40 mm/yr \cite{3} with the potential consequence to favor significant intrusion of seawater into potable coastal aquifers \cite{4} and groundwater flooding of urban areas \cite{5} and infrastructure. Despite some indicators of the interaction between infrastructures with urban coastal aquifers, few studies have been dedicated to develop methods and models to quantify this interaction \cite{6,7}.

Here, we report a study to investigate the interaction of a coastal urban aquifer with a sewer network. The area (Hoboken, NJ) is located in the North-East of the United States at the Hudson river estuary within the metropolitan area of New York city. The work was motivated by large concentration of fecal indicator bacteria in the river during dry weather suggesting groundwater inundation of the sewer. The watershed was implemented in MODFLOW with a geology determined by applying geostatistics on few localized geological data. Boundary data consisted of variable aquifer head and tidal river level. The hydraulic conductivity and the recharge were estimated through stochastic inverse modeling on the hydraulic head measurements within the domain of interest. By knowing the location of the sewer pipes and compared with the estimated groundwater table with uncertainty, the potential of groundwater inundation of the sewer was assigned to each part of the network.

References:
Reference
\textsuperscript{2} Owolabi Glob. Ini., 11, 69-87, 2017
\textsuperscript{3} Milne Astro. Geophys., 49, 224-228, 2008
\textsuperscript{5} Kane, H. H., ets. Reg. Environ Change, 15(8), 1679–1687
\textsuperscript{7} Karpf and Krebs. Water Research, 45, 3119-3136, 2011  Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-B / 589

Use of Biogenic Gas Production as a Pre-Treatment to improve the Efficiency of Dynamic Compaction

Author(s): Devajani Borah\textsuperscript{1}

Co-author(s): Leon Van Paassen \textsuperscript{2}; Kavazanjian Edward \textsuperscript{1}
One of the most economical and viable methods of soil improvement is dynamic compaction. However, dynamic compaction can only be applied on deposits where the degree of saturation is low and the permeability of the soil mass is high to allow for good drainage. The technique does not work very well on soils having a large content of fines. Also dynamic compaction produces lateral ground vibrations which can travel far from the construction site, which can discomfort the people living close to these areas. The current research aims to develop a new technology to desaturate saturated soils using the process of MIDP – Microbially Induced Desaturation and Precipitation through nitrate reduction, which extend the use of dynamic compaction as a ground improvement technique to saturated soil conditions and soils with higher fines content. To evaluate the feasibility of this technology an experimental program has been performed, in which soil columns have been treated with MIDP. In this process, indigenous micro-organisms are stimulated to convert nitrate into nitrogen gas, which desaturates the soil. After the process has finished, dynamic loading is applied to the soil columns. During the MIDP process and during the dynamic loading, the deformation and pore pressure area measured for various amounts of compactive effort and compared with the non-treated soil. Based on the experimental results the feasibility of the proposed technology is discussed.

References:
Pham, V. P. (2017), Bio-based Ground Improvement through Microbial Induced Desaturation and Precipitation (MIDP), PhD thesis, Technical University Delft.

Acceptance of Terms and Conditions:
Click here to agree

Parallel 9-G / 41

Use of Lagrangian coherent structures and angular multiscale statistics to assess turbulence in porous media

Sourabh Apte1; Justin Finn2; Xiaoliang He1

1 Oregon State University
2 1) National Energy Technology Laboratory, Albany, OR. 2) AECOM, Albany OR.

Corresponding Author(s): sva@oregonstate.edu

Two approaches based on Lagrangian statistics of turbulent flow in porous media are investigated. In the first approach, usage of Lagrangian coherent structures (LCS) to understand barriers in transport and mixing in turbulent flows is studied. The computation of LCS typically involves post processing of experimentally or numerically obtained fluid velocity fields to obtain the finite time Lyapunov exponent (FTLE) via a sequence of flow maps (vector fields which describe fluid displacement patterns over a finite time interval). However, this procedure can be prohibitively expensive for large-scale complex flows of engineering interest. In this work, an alternative and efficient approach involving computation of the FTLE on the fly during direct numerical simulation (DNS) of the 3D Navier-Stokes equations is developed. Spatio-temporal evolution of LCS in a turbulent flow in a randomly packed porous bed are computed, and their role in identifying dead zones, mixing length and time-scales are assessed. In the second approach, Lagrangian statistics of scale dependent curvature angle and acceleration are calculated by tracking a large number of fluid particle trajectories for turbulent flows in porous media over a range of Reynolds numbers (300-1000). For an isotropic turbulence, it
has been shown that the mean curvature angle varies linearly with time initially, reaches an inertial range and asymptotes to a value of $\pi/2$ at long times, corresponding to the decorrelation and equipartition of the cosine of the curvature angle. Similar trends are observed at early times for turbulence in porous medium; however, the mean curvature angle asymptotes to a value larger than $\pi/2$. This is attributed to the effect of confinement on the fluid particle trajectories that result in preferred directions at large times. The two Lagrangian approaches and their importance in analysing turbulence and transport in porous media will be illustrated.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-E / 14

Use of molecular simulations to fit EOS in confined space in order to perform large scale tight oil and shale gas reservoir simulations

Nicolas Sobecki$^1$ ; Didier Ding$^1$ ; Carlos Nieto-Draghi$^1$ ; Yu-Shu Wu$^2$

$^1$ IFPEN

$^2$ Colorado School of Mines

Corresponding Author(s): nicolas.sobecki@ifpen.fr

Unlike conventional reservoirs where pore size distribution has a micrometer scale (Nelson 2009), tight oil and shale gas reservoirs have predominantly mesopores (between 2 and 50 nm) and micropores (below 2 nm). Volume fraction of micropores is not negligible and can be as high as 20% (Kuila et Prasad 2011). As hydrocarbon molecules range between 0.5 and 10 nm (Nelson 2009), interaction forces between confined fluid and pore wall molecules become as significant as inter molecular interactions within the confined fluid. That is why nanofluidic experiments (Wang et al. 2014) and bubble point measurement on hydrocarbon mixture in mesoporous materials (Cho, Bartl et Deo 2017) have demonstrated that confinement considerably changes fluid phase behavior. Consequently the commonly-used equation of state (EOS) such as Peng-Robinson EOS is not able to describe the confined fluid phase behavior. A pore radius dependent EOS is therefore needed in reservoir simulators for accurate large scale tight oil and shale gas production forecast simulations.

The idea of this work is to integrate first the capillary pressure effect into the classical Peng-Robinson EOS and then to calibrate EOS parameters function of pore radius to fit molecular simulations. The capillary pressure which depends on pore radius adds pressure difference between vapor and liquid phase in the equilibrium computation. It is calculated using the Young-Laplace equation. Molecular simulation is performed using Monte Carlo method in the grand canonical and in the NVT Gibbs ensemble with anisotropic volume change in order to calculate equilibrium properties of several pure hydrocarbon components and mixtures in confinement. Kerogen pores are modelled by graphite slit pores and fluid/wall interaction potential is added. For a given pore radius, the critical temperature and pressure are determined for pure components, and liquid and vapor pressures, densities and molar fractions of components are calculated for both pure components and mixtures at different temperatures for calibration. These values are used as reference fitting data for the Peng-Robinson EOS with capillary pressure. The optimization parameters are the Peneloux volume correction constant, the acentric factor and the binary interaction coefficients. The calibration of these parameters allows getting correlations versus pore radius that will be used to model the confined fluid thermodynamic behavior.

The pore radius dependent EOS calibrated with molecular simulation data can therefore be used in reservoir simulators to accurately forecast tight oil and shale gas production. However the grid cells in a dynamic flow simulation is usually in order of several meters to 100m. Such a cell includes a large pore size distribution, the pore radius value used in the EOS is therefore an issue. In order to consider the pore size variability within a simulation cell, an effective radius function of oil saturation
is taken. It is determined from the distribution function of pore size volume. Assuming oil is the wetting phase, during a flow simulation, oil is present in small pores and gas appears in larger pores, then the effective pore radius decreases. Oil and gas production simulations with a dual porosity model for a fractured tight-oil reservoir show that this methodology gives more reasonable results than using an average pore radius and of course than a bulk approach.

References:


Wang, Lei; Parsa, Elham; Gao, Yuefeng; Ok, Jeong Tae; Neeves, Keith; Yin, Xiaolong; Ozkan, Erdal (2014) Experimental Study and Modeling of the Effect of Nanoconfinement on Hydrocarbon Phase Behavior in Unconventional Reservoirs. SPE Western North American and Rocky Mountain Joint Meeting. DOI: 10.2118/169581-MS

Accepted Terms and Conditions:

Click here to agree

Invited 3 (Room D) - Dorthe Wildenschild / 1110

Using 3D Microimaging to Evaluate the Effect of Nutrient Flow Rate on Biofilm Growth in Porous media

Author(s): Dorthe Wildenschild¹

Co-author(s): Sassan Ostvar ; Gabriel Itlis ; Yohan Davit ; Steffen Schlüter ; Linnéa Andersson ; Brian Wood

¹ Oregon State University

Corresponding Author(s): dorthe@engr.oregonstate.edu

We use microimaging to study the effects of flow rate on three-dimensional growth of biofilm in porous media. Three flow rates were investigated in model packed-bed columns, while biofilm was grown over a period of 11 days. At the end of the growth period, all columns were scanned using x-ray computed microtomography and a barium sulfate-based contrast agent to distinguish the biofilm. We used differential pressure transducer and effluent dissolved oxygen measurements to complement and validate the image-based findings. Reduction in permeability due to biofilm growth was studied using both transducer-based pressure drop measurements and image-based calculations using the Kozeny-Carman model. A combination of results from these different measurements suggest that biofilm growth was oxygen limited at the lowest flow rate, and affected by shear stresses at the highest flow rate. We hypothesize that the interplay between these two factors drives the spatial distribution and quantity of biofilm growth in the class of porous media studied here. Our approach opens the way to more systematic studies of the structure-function relationships involved in biofilm growth in porous media and the impact that such growth may have on physical properties such as hydraulic conductivity.

References:

Accepted Terms and Conditions:

Click here to agree

Parallel 6-D / 686

Using Micromodels to Study Heavy Oil Displacement by Foam
Eric Vavra¹ ; Lisa Biswal¹ ; George Hirasaki¹

¹ Rice University

Corresponding Author(s): edv1@rice.edu

Micromodels are a proven platform for offering new insights into the area of foam enhanced oil recovery (EOR). These tools provide us with not only analytical information for the characterization of particular oil-surfactant systems but also allow us to gain fundamental insight into the mechanisms that drive the oil displacement process. In addition, the polymer-based micromodels we use offer a combination of organic solvent resistance, reproduction of physical rock properties, and ease of manufacturing. In this talk, I will discuss our recent work using micromodels to visualize and probe the mechanisms of heavy crude oil displacement by surfactant-stabilized foams. On the pore-scale, we observe several key mechanisms that lead to high oil displacement even at low capillary numbers. Interfacial interactions, wettability alteration, foam generation, and foam destruction were all phenomena of interest in our experiments. Using micromodels, we are able to gain new information about our oil recovery platform and ultimately improve upon our understanding of how to design effective foam-flooding strategies.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-F / 753

Using Nanofluids to Control Fines Migration for Oil Recovery: Nanofluids Co-injection and Nanofluids Pre-flush

Bin Yuan¹

¹ University of Calgary (previous at University of Oklahoma))

Corresponding Author(s): ybpetro1990@gmail.com

This work provides a comprehensive study to evaluate and optimize the effectiveness of nanofluids to both prevent fines migration and enhance oil recovery using different utilization approaches: nanofluids co-injection and pre-flush. To do that, 1) a comprehensive review of both laboratory experiments and field cases is adopted to confirm the effectiveness of nanoparticles to control fines migration. 2) A novel model of maximum fines retention concentration is then introduced to find out the physical mechanisms on how nanoparticles control fines migration. 3) Through matching with lab experiments, the physical behaviors of fines migration and attachment with the effects of different types of nanofluids are characterized, including fines attachment and straining rates, and breakthrough time of injected fines. 4) As a new criterion, mitigation index (MI) is defined to find out the more excellent performance of nanofluids pre-treatment that that of nanofluids co-injection. 5) In two-phase oil/water flow, analytical modeling and solutions of nanoparticles to control fines migration is developed, in terms of both enhanced oil recovery and well injectivity. 6) The pros and cons of fines migration on performance of low-salinity water flooding are discussed comprehensively, in this work, and the success of combining nanofluids with low-salinity water flooding is also confirmed to achieve more oil recovery. The outcomes of this work will help extend the applications of nanofluids in reservoirs suffering from problems of fines migration.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 10-D / 889
Using Surfactants to Induce Viscosity Driven Crossflow in Oil-Wet Fractured Micromodels

Author(s): Lucas Mejia

Co-author(s): Matthew Balhoff; Ke Xu; Mohsen Tagavifar

1 The University of Texas at Austin
2 University of Texas at Austin

Corresponding Author(s): lmkerguelen@utexas.edu

The objective of this work is to use micromodels to investigate the feasibility of using viscous microemulsions to mobilize oil in fractured, oil-wet porous media by inducing crossflow. Production by water flooding from fractured oil-wet media, such as carbonates, is challenging because capillary forces prevent water imbibition into the matrix. Recently, experimental core floods (Parra et al., 2016) and numerical simulation (Abbasi et al., 2010) have demonstrated extremely high recoveries in carbonates even with fracture/matrix permeability ratios above 10,000 by using surfactants to reduce the interfacial tension and create in-situ viscous microemulsions to create transverse pressure gradients. Here, we conducted low IFT floods in oil-wet, fractured glass micromodels to show that the recovery is due to crossflow, the recovery is significant (30-40% OOIP after flooding for 1 pore volumes), microemulsions are formed and visible, and a cone-shaped sweep pattern is consistent with reservoir simulation studies. We also show that the rate of crossflow is dependent on the viscosity of the microemulsion.

A glass micromodel was fabricated using conventional photolithography procedures. The micromodel has a fracture with permeability 1000 times greater than the matrix. To make the micromodel oil-wet, the glass surface was activated with sulfuric acid, silylated with an alkylsilane, and aged in oil.

The micromodels were saturated with low viscosity (13 cp) light oil and water flooded for several pore volumes until no reduction in oil saturation was observed. Immediately following the water flood a surfactant solution with low IFT was injected continuously. Surfactant slugs of different salinities, but all at low IFT, were injected to investigate the role of microemulsion viscosity on oil recovery. Image sequences of the floods were captured and analyzed using ImageJ for changes in saturation versus time.

Waterflooding the micromodel only resulted in production in the fracture because large capillary forces prevent water imbibition into the matrix. However, we observed significant crossflow and production from the matrix when surfactant solution was injected for 0.5 pore volumes. The micromodels were flat, so buoyant forces were negligible and all the crossflow was from transverse, viscous pressure gradients. The in-situ microemulsion viscosity was controlled by salinity and we show that higher viscosities (e.g. 50 cp versus 13 cp) result in higher recoveries. The sweep pattern is approximately “cone shaped” as predicted in numerical simulation.

The following was observed from the experiment:
• Crossflow in 2D and 2.5D fractured, oil-wet micromodels was observed when viscous microemulsions were formed in-situ to create transverse pressure gradients.
• Production from the matrix occurred in the same cone-shaped patterns as predicted by reservoir simulation.
• Higher recoveries were achieved using higher viscosity microemulsions, created by varying salinity.

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 4-F / 757

Vanishing artificial capillary pressure as a mechanism to accelerate convergence

Pablo Salinas¹; Christopher Pain¹; Hossam Osman¹; Dimitrios Pavlidis¹; Zhilhua Xie¹; Matthew Jackson¹

¹ Imperial College London
² Cardiff University

Corresponding Author(s): pablo.salinas@imperial.ac.uk

Modelling multiphase porous media flows is important in many engineering areas such as geothermal energy extraction, unconfined aquifers, CO₂ storage, magma reservoirs and hydrocarbon reservoirs. However, modelling of multiphase porous media flow is very challenging due to various reasons: the relative permeabilities (controlled by the saturation) introduces high non-linearities in the system; physical diffusion (a very stabilising term) does not appear in the equations, only when capillary pressure is present a diffusive effect appears in the flow. However, it is also controlled by the saturation, further increasing the non-linearity of the system. Controlling these non-linearities through the non-linear solver is very important to be able to obtain stable solutions with Courant numbers that allow to model real size reservoirs in an acceptable period of time.

A common approach to stabilise the system arising from the discretisation of the advection equation is to introduce artificial diffusion. However, introducing artificial diffusion does change the result, therefore a balance has to be found so that the introduced artificial diffusion is strong enough so it helps to solve the system while not severely affecting the final result.

In Salinas et al. 2017, a vanishing artificial diffusion was detailed. In that method, the diffusion was controlled by the convergence of the non-linear solver by multiplying the artificial diffusion term by the difference between the most recent saturation estimation and the one obtained in the previous non-linear iteration. This method allows to use higher artificial diffusions while also minimising the artificial diffusion effect in the result. Nonetheless, as the saturation estimation from the previous non-linear iteration is introduced in the right-hand side of the equations, if the difference between saturation estimations when the non-linear solver has converged is not small enough, then a source/sink term is introduced for that specific phase.

Here, a conservative vanishing artificial diffusion is presented. It improves the convergence and convergence rate of the non-linear solver by reducing the non-linearity of the equations. Moreover, it is tailored to specially help to deal with the capillary pressure. The vanishing artificial diffusion is introduced using the same model employed to introduce the capillary pressure, obtaining a vanishing artificial capillary pressure diffusion term. By introducing this vanishing artificial diffusion in the saturation equation, which is solved implicitly, a very efficient method to model multiphase porous media flow with physical capillary pressure is obtained. This method provides accurate results and significantly reduces the effort required by the non-linear solver to achieve convergence. It enables to carry out very demanding numerical simulations, e.g. when the capillary pressure effects are dominant, with Courant numbers that are at least two orders of magnitude bigger than without it. For this particular case, it enables to obtain solutions up to 175 times faster than before.

References:

References:

Acceptance of Terms and Conditions:
Click here to agree
Parallel 1-A / 345

Vertically-Integrated Dual-Continuum Models for CO2 Injection in Fractured Saline Aquifers

Author(s): Yiheng Tao
Co-author(s): Bo Guo ; Karl Bandilla ; Michael Celia

1 Princeton University
2 Stanford University

Corresponding Author(s): yihengt@princeton.edu

Injection of CO2 into a saline aquifer leads to a two-phase flow system, including a supercritical CO2 phase and a brine phase. Various modeling approaches, including fully three-dimensional (3D) models and vertical-equilibrium (VE) models, have been used to study the system in unfractured formations. Three-dimensional models solve the governing flow equations in three spatial dimensions and are applicable to generic geological formations. VE models assume rapid and complete buoyant segregation of the two fluid phases, resulting in vertical pressure equilibrium and allowing integration of the governing equations in the vertical dimension. This reduction in dimensionality makes VE models computationally much more efficient, but the associated assumptions restrict the applicability of VE model to formations with moderate to high permeability.

In this presentation, we extend the VE and 3D models to simulate CO2 injection in fractured aquifers. This is done in the context of dual-continuum modeling, where the fractured formation is modeled as an overlap of two continuous domains, one representing the fractures and the other representing the rock matrix. Both domains are treated as porous media continua and, as such, can be modeled by either a VE or a 3D formulation. The transfer of fluid mass between fractures and rock matrix is represented by a mass transfer function connecting the two domains. Because the fracture domain is usually much more permeable than the matrix domain, we apply VE modeling to the fracture domain but not the matrix domain. We refer to the resulting model as a hybrid VE-3D model, with the VE model applied to the highly permeable fractures and the 3D model in the less permeable rock matrix.

Our hybrid VE-3D model includes both dual-porosity and dual-permeability types. The dual-porosity model conceptualizes the rock matrix as sugar-cubes that are isolated uniformly by vertical and horizontal fractures, or as matchsticks that are isolated by vertical fractures through the entire thickness of the aquifer. In contrast, the dual-permeability model explicitly represents the 3D flow dynamics in the rock matrix. We derive mass transfer functions that couple the VE model in the fracture to the different models in the rock matrix. We then apply the hybrid VE-3D model to simulate CO2 migration in fractured saline aquifers and compare with 3D-3D models where both the fracture and rock matrix are modeled in 3D. The hybrid VE-3D models are much more computationally efficient while providing results that are close to those from the 3D-3D models. These vertically-integrated dual-porosity and dual-permeability models provide a range of computationally efficient tools to model CO2 storage in fractured saline aquifers.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 5-A / 513

Viscous fingering and nonlinear waves in a Langmuir adsorbed solute

Author(s): Chinar Rana
Co-author(s): Michel Martin ; Satyajit Pramanik ; Manoranjan Mishra ; Anne De Wit
Waves in chromatography are well known to the practitioners. Characteristics of these waves are strongly correlated to the nature of the adsorption isotherm. We model the displacement of a finite slice containing an adsorbed solute by a carrier liquid flow. We examine the nonlinear dynamics that emerge from the interactions of rarefaction, shock layer and/or viscous fingers (VF) in the finite solute slice that adsorbs on a porous matrix according to a Langmuir isotherm. The differences between a linear and a Langmuir isotherm are discussed. In the absence of VF, a shock layer (rarefaction) wave appears at the frontal (rear) interface of the solute. VF at a viscously unstable rarefaction interface propagates through the finite sample to preempt the shock layer. However, no such incident is observed when the shock layer front features VF. Various quantities (e.g., the onset of VF, shock layer thickness, etc.) are calculated as a function of the saturation rate and the results are supported by mathematical analysis.

References:

Acceptance of Terms and Conditions:
Click here to agree

Viscous fingering with partially miscible fluids

Xiaojing Fu\(^1\); Luis Cueto-Felgueroso\(^2\); Ruben Juanes\(^3\)

\(^1\) Massachusetts Institute of Technology
\(^2\) Technical University of Madrid, Madrid, Spain
\(^3\) MIT

Corresponding Author(s): rubyfu@mit.edu

Viscous fingering—the fluid-mechanical instability that takes place when a low-viscosity fluid displaces a high-viscosity fluid—has traditionally been studied under either fully miscible or fully immiscible fluid systems. In practice, however, the miscibility between two fluids can change appreciably with temperature and pressure and often falls into the case of partial miscibility, where two fluids have limited (but nonzero) solubility in each other (e.g. CO\(_2\) and water). Following our recent work for miscible systems \([1, 2]\) and immiscible systems \([3, 4]\), here we study the impact of partial miscibility on the pattern forming dynamics of viscous fingering \([5, 6]\). Through a careful design of the thermodynamic free energy of a binary mixture, we develop a phase-field model of fluid-fluid displacements in a Hele-Shaw cell for the general case in which the two fluids have limited (but nonzero) solubility into one another \([5]\). We show, by means of high-resolution numerical simulations, that partial miscibility exerts a powerful control on the degree of fingering: fluid dissolution hinders fingering while fluid exsolution enhances fingering. We also show that, as a result of the interplay between compositional exchange and the hydrodynamic pattern-forming process, stronger fingering promotes that the system approach thermodynamic equilibrium faster.

References:


Acceptance of Terms and Conditions:
Parallel 2-A / 343

Visualisation of solute transport and determination of its transport properties in porous sintered glass

Author(s): Stefanie Van Offerenw1
Co-author(s): Tom Bultreys2; Jeroen Van Stappen1; Marijn Boone3; Veerle Cnudde1

1 Ghent University, Pore-scale Processes in Geomaterials Research Team (PProGRess)
2 Department of Earth Science and Engineering, Imperial College London
3 XRE NV

Corresponding Author(s): stefanie.vanofferenw@ugent.be

Solute transport in porous media is important for several industrial applications, i.e.: hydrology, building stone performance and waste management. Spreading and mixing during solute transport is significantly impacted by the pore scale heterogeneity found in natural porous media, which complicates upscaling (Dentz et al., 2011). Therefore, simulations and experiments which investigate the evolution of pore scale solute concentration fields in such materials are very valuable. However, direct visualisation of these concentration fields at the micron-scale in rocks is complicated by the high spatial and time resolutions that are required. Bultreys et al. (2016) and Boone et al. (2016) present first tests on imaging solute transport in a carbonate rock using fast laboratory-based micro-CT. In this study, we extend this work by attempting to quantify micro-CT concentration fields, in order to investigate spreading and mixing under different flow conditions in porous materials with different degrees of heterogeneity.

A significant part of this work is aimed at the methodological challenge of performing in-situ micro-CT scans of solute transport with imaging times on the order of seconds. We use the EMCT scanner of UGCT (www.ugct.ugent.be), a micro-CT system specially designed for in-situ imaging, with a rotating X-ray tube and detector in a horizontal plane (Dierick et al., 2014) and investigate the quantitative correctness when imaging the concentration of a dissolved tracer salt (0 wt%, 2 wt%, 4 wt%, 6 wt%, 8 wt% and 10 wt% CsCl) in porous sintered glass at 12 seconds per scan, with a voxel size of 13 micron. The CsCl-concentration increases the X-ray attenuation coefficient of the fluid, which causes an increase in grey values observed in the reconstructed micro-CT datasets. The high temporal resolution at which the micro-CT images are taken, is inherently linked with a limited signal-to-noise ratio. Despite this drawback, the first experimental results suggest a linear relationship between the grey values of the tracer-solution in the fast scans and the tracer concentration.

Results from the presented experiments can be used to investigate flow structures at the pore scale and to validate pore scale solute transport simulations. Further development of the methodology could also lead to valuable insights in multi-phase solute transport and reactive transport.

References:
Boone, M., Bultreys, T., Masscheele, B., Van Loo, D., Van Hoorebeke, L. & Cnudde, V., 2016. In-situ real time micro-CT imaging of pore scale processes, the next frontier for laboratory based micro-CT scanning. Paper was prepared for presentation at the International Symposium of the Society of Core Analysts held in Snowmass, Colorado, USA, 21-29 August 2016.
Visualization of flows in 3D-printed fractured porous media: an experimental approach

Author(s): Mehrdad Akhami¹ ; Anozie Ebigbo²
Co-author(s): Thomas Roesgen³ ; Martin O. Saar¹ ; Xiang-Zhao Kong¹

¹ Institute of Geophysics, ETH Zurich
² ETH Zurich
³ Institute of Fluid Dynamics, ETH Zurich

Corresponding Author(s): anozie.ebigbo@erdw.ethz.ch

In-depth understanding of fluid and solute transport through complex porous media is of significant importance in various engineering and scientific applications. Large-scale behaviour of fluid and solute transport are determined by pore-scale features. Therefore, it is crucial to determine pore-scale transport properties and then upscale these properties to large scales. Numerically lattice-Boltzmann methods (LBM) have shown the potential to simulate flow in porous media with high Knudsen numbers. On the other hand, a limited number of experimental studies have been proposed, and even less actually conducted, to characterize pore-scale flow in porous media with sufficient spatial resolution to test or verify numerical results.

Recent advances in 3D-printing technology offer the capability to precisely manufacture transparent fractured porous media, enabling optical flow visualization employing, for example, Particle Shadow Shadow Velocimetry (PSV). In this study, the flow is optically visualized in a transparent fractured porous medium with two flow-through and two dead-end fractures, symmetrically embedded in two matrices with different pore sizes. This medium is designed to represent dual-permeability, dual-porosity porous systems. A LED light source was used to back-illuminate the flow chamber and a monochrome camera was used to record image sequences of the seeded flow through the fractured porous medium. Flow velocities were determined by local pattern cross-correlation. Measured velocities were compared with LBM simulations, performed for the same porous medium geometry. Our results demonstrate the potential of using quantitative flow visualization techniques to characterize fluid flow in complex porous systems.

References:

Acceptance of Terms and Conditions:
Click here to agree

Visualizing and Quantifying Biominalization in a Wellbore Analog Reactor

Drew Norton¹ ; Catherine Kirkland¹ ; Robin Gerlach¹ ; Joe Eldring¹ ; Al Cunningham² ; Lee Spangler¹ ; Adrienne Phillips¹

¹ Montana State University
² Center for Biofilm Engineering, Montana State University

Corresponding Author(s): adrienne.phillips@montana.edu

Subsurface fluid injection is a proposed method for the storage of hydrocarbon fuels and the mitigation of fossil fuel emissions. Concerns about leakage exist when storing fluids in the subsurface given their potential to damage functional groundwater aquifers or be emitted to the atmosphere.
Defects detrimental to the integrity of subsurface storage systems can occur in and around the wellbore, thus fluid storage systems are heavily dependent on the cement surrounding the wellbore to maintain a seal.

A method proposed to seal defects in the subsurface is Microbially Induced Calcium Carbonate Precipitation (MICP). MICP is a technique that uses low viscosity fluids and microorganisms (~2 μm diameter) to seal defects troublesome to subsurface fluid storage. In the MICP process, microorganisms such as Sporosarcina pasteurii that contain the enzyme urease catalyze the hydrolysis of urea to produce ammonium and carbonate species. When this process occurs in the presence of dissolved calcium, calcium carbonate may precipitate.

To study MICP in defects common to the wellbore, two reactors systems were created. The first was constructed to mimic the geometry of the wellbore and allowed the visual observation of MICP formation. The second quantified MICP in a cement channel defect using X-ray computed microtomography. A reduction in apparent permeability and void fraction was observed in both systems, demonstrating the ability of MICP to restrict fluid flow in defects common to the wellbore. Observations made during these experiments will aid in improving the safety and efficacy of subsurface fluid storage systems.

References:
Acceptance of Terms and Conditions:
Click here to agree

Poster 3 / 640

Visualizing and studying Multiphase flow in ITO coated micro-capillary.
Chike Ezech1; Chia-Yu Chen1; Kyriakos Papadopoulos1

1 Tulane University

Corresponding Author(s): cezech@tulane.edu

A technique for studying flow in porous media at the lab scale has been previously developed in our laboratory. The technique involves a confined miniature cylindrical geometry that is obtained by heating and pulling on a 100ml cylindrical capillary. The narrow region of the capillary, tapered and cylindrical, is filled with cryolite to form a random, porous medium, and two-liquid-phase-flow experiments are conducted in this region. This experimental setup offers unique and novel ability to monitor two-phase flow in a transparent random porous medium in real-time. Also, the images and videos obtained from this experimental setup can be analyzed to obtain useful information, such as the flow pattern, oil mobilization efficiency, and hydraulic conductivity. In the present work, a thin film of Indium Tin Oxide(ITO) is coated on the outside of the capillary to render the capillaries electrically semi-conductive. By applying electric current to the outside of the coated capillary, the temperature of the capillary is elevated, and two-phase-flow experiments at elevated temperatures are conducted in the porous medium.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-B / 145

Water management of plant tissues during frost-thaw cycles
Lukas Eurich1; Arndt Wagner1; Wolfgang Ehlers1
Plant tissues have developed several strategies to cope with multiple cycles of freezing and thawing events without being damaged. Some of these strategies are of physiological nature, others arise from structural properties. Understanding the involved strategies and mechanisms of plants exposed to frost conditions is of high interest, as they could potentially be used for the development of bio-inspired construction materials with optimised properties in terms of frost resistance, thermal isolation and guided water/moisture transport.

A decisive factor with regard to frost resistance in plants is the dehydration of the tissue cells leading to an increase of mobile water in the intercellular space. In contrast, freezing within the cells threatens the survivability of the plant. The intercellular water is then transported to species-specific and tissue-specific locations in the plant where freezing is not critical. For this water management, properties of the plant’s microstructure are crucial, which are arising from the arrangement of the tissue cells. This arrangement results in highly heterogeneous and anisotropic conditions. Particularly the role of these structural effects is of interest for a transfer to construction materials.

Since the involved thermo-hygro-mechanical processes in plant tissues upon freezing and thawing cycles are strongly coupled, a modelling approach based on the Theory of Porous Media (TPM) is applied, which describes the multiphasic and multicomponent aggregate on the macroscale. In particular, a quaternary model is introduced with a solid skeleton (composed of the tissues cells) and two fluids in the intercellular space, namely, gaseous air and liquid water, which may turn into solid ice. The phase transition of water occurs at a singular surface, which is characterised by a jump in physical quantities, such as the density. The mass transfer can be formulated by using the energy jump at this interface leading to a thermodynamically consistent formulation. In this approach, the interfacial area between liquid and solid water in the partially saturated plant tissues needs to be considered. The freezing of the pore water leads to the necessity to consider the so-called compaction point in the material description, as the bulk material undergoes a transition from a porous material to a solid material. Furthermore, the cell dehydration is included by a production term in the mass balance of the solid skeleton using a Darcy-type law for the cell-wall perfusion. A similar Darcy-type approach was chosen for the fluid flow within the intercellular space with spatially varying anisotropic permeability conditions enabling, thereby, a description of the water management. All these effects are illustrated by selected numerical examples.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 8-G / 782

Weak Galerkin Method and Its Applications

Xiu Ye

Corresponding Author(s): xxye@ualr.edu

Newly developed weak Galerkin (WG) finite element methods will be introduced for solving partial differential equations on polygonal mesh. The weak Galerkin method is a natural extension of the standard Galerkin finite element method for the function with discontinuity where classical derivatives are substituted by weakly defined derivatives. Therefore, the weak Galerkin methods have the flexibility of employing discontinuous elements and, at the same time, share the simple formulations of continuous finite element methods.

The purpose of this presentation is to introduce some new developments of the WG methods and their applications. A robust WG method will be presented for solving the Reissner-Mindlin plate
problem with uniform convergence. Also a simple WG method will be introduced to solve for singularly perturbed convection-diffusion-reaction problems. A posteriori analysis with simple estimator for WG method will also be discussed.

References:
Acceptance of Terms and Conditions:
Click here to agree

Parallel 3-H / 911

Wettability and Quasi-Static Fluid-Fluid Displacement in Micromodels

Bauyrzhan Primkulov\textsuperscript{1} ; Stephen Talman\textsuperscript{2} ; Rick Chalaturnyk\textsuperscript{2} ; Keivan Khaleghi\textsuperscript{2} ; Alireza Ranriz Shokri\textsuperscript{2} ; Robin Zhao\textsuperscript{3} ; Christopher MacMinn\textsuperscript{4} ; Ruben Juanes\textsuperscript{1}

\textsuperscript{1} MIT
\textsuperscript{2} University of Alberta
\textsuperscript{3} Massachusetts Institute of Technology
\textsuperscript{4} Oxford U.

Corresponding Author(s): bprimkul@mit.edu

Wettability of porous media has a remarkable influence on the morphology of invading fronts during fluid-fluid displacement. For example, it has been shown that when invading and defending fluids exhibit an instability-inducing viscosity ratio, the invading phase advances through viscous fingering, and the width of the fingers is dictated by the substrate wettability. When the porous medium has low affinity to the invading liquid (drainage), the width of the fingers is comparable to a pore size. In contrast, when the porous medium has high affinity to the invading liquid (imbibition), the thickness of the fingers is well above the pore size, and the invading phase advances as a more smooth and compact front [1, 2]. Recently, the experimental observations were extended to the strong imbibition regime. It was shown that, in this case, front displacement occurs via corner flow, where the invading fluid advances by coating the posts in a patterned Hele-Shaw cell [3].

Motivated by these experimental observations in patterned microfluidic cells, we build on the work of Cieplak and Robbins [3] to develop a quasi-static pore invasion model for the full range of pore wettabilities, from strong drainage to strong imbibition. We describe the pore geometry as a pore network, and explicitly calculate the critical pressures of pore invasion events to advance the fluid-fluid interface based on these pressure thresholds. This revisited formulation of fluid invasion removes the bias associated with user-dependent choices of pressure increments during the invasion, or conventions for the sequence of interface pore configurations. Our quasi-static simulations show a transition from invasion-percolation to cooperative pore filling to corner flow as the wettability of the medium to the invading fluid increases, in quantitative agreement with the experimental observations on micromodels.

Finally, we extend our model from a quasi-static to a dynamic description by accounting for viscous forces during pore invasion, and buoyancy effects from density difference between the fluids. We apply the new model to investigate impact of wettability on the morphology of unstable flow during secondary oil migration.

References:
Parallel 8-F / 210

Wettability and flow rate impacts on immiscible displacement: a theoretical model

Ran Hu1; Yi-Feng Chen1; Zhibing Yang1

1 Wuhan University

Corresponding Author(s): whuran@whu.edu.cn

When a more viscous fluid displaces a less viscous one in porous media, viscous pressure drop stabilizes the displacement front against capillary pressure fluctuation. For this favorable viscous ratio conditions, previous studies focused on the front instability under slow flow conditions but did not address competing effects of wettability and flow rate. Here we study how this competition controls displacement patterns. We propose a theoretical model that describes the crossover from fingering to stable flow as a function of invading fluid contact angle \( \theta \) and capillary number \( Ca \). The phase diagram predicted by the model shows that decreasing \( \theta \) stabilizes the displacement for \( \theta \leq 45^\circ \) and the critical contact angle \( 0c \) increases with \( Ca \). The boundary between corner flow and cooperative filling for \( \theta < 45^\circ \) is also described. This work extends the classic phase diagram, and has potential applications in predicting CO2 capillary trapping and manipulating wettability to enhance gas/oil displacement efficiency.

References:


Parallel 4-H / 855

Wettability control on multiphase flow in porous media: A benchmark study on current pore-scale modeling approaches

Ruben Juanes1; Benzong Zhao2; Christopher MacMinn3

1 MIT
2 U. Toronto
3 Oxford U.

Corresponding Author(s): juanes@mit.edu

Multiphase flow in porous media is important in many natural and industrial processes, including geologic CO2 sequestration, enhanced oil recovery, and water infiltration into soil. Although it is well known that the wetting properties of porous media can vary drastically depending on the type
of media and pore fluids, certain aspects of wettability control on multiphase flow continue to challenge our microscopic and macroscopic descriptions. The gap in our understanding could be bridged by pore-scale modeling, which has seen rapid development in recent years and is becoming a useful predictive tool in both academic and industrial applications. The goal of this work is to validate and improve different pore-scale modeling methodologies by comparing the modeling results from various leading researchers with a benchmark experimental dataset on patterned microfluidic cells. As part of the benchmark study, we received submissions from over 10 research groups from around the world, whose modeling approaches include Lattice Boltzmann methods (LBM), smoothed particle hydrodynamics (SPH), Cahn-Hilliard phase-field models, volume of fluid (VoF) methods, level-set methods (LSM), and pore-network models. For each submission, we conduct both qualitative and quantitative comparisons between the modeling results and the experimental results. Qualitatively, we compare the macroscopic fluid-fluid displacement patterns for a given wettability condition and capillary number. Quantitatively, we compare the fractal dimension of the displacement pattern, the median saturation, and the displacement efficiency of the invading fluid. Despite the high computational demand of simulating the fluid-fluid displacement process at the pore-scale, the modeling results have shown impressive agreement with the experiments. In particular, most modeling approaches are able to capture the increasingly compact displacement pattern in the transition from strong drainage (i.e. highly non-wetting invading fluid) to weak imbibition (i.e. weakly wetting invading fluid). However, capturing the flow behavior in strong imbibition (i.e. highly wetting invading fluid) proves to be much more challenging. This is because strong imbibition is dominated by capillary-assisted corner flow, where the 3D configuration of the fluid-fluid interface is important. The present study highlights the need to develop alternative pore-scale modeling methodologies capable of accounting for the 3D nature of interfacial flows in a computationally efficient manner.

References:


Click here to agree

Parallel 7-D / 887

Wetting, disorder, and pattern formation

Author(s): Amir Pahlavan

Co-author(s): Luis Cueto-Felgueroso ; Gareth McKinley ; Ruben Juanes

MIT

Technical University of Madrid, Madrid, Spain

Corresponding Author(s): pahlavan@mit.edu

In their seminal work, Saffman and Taylor showed that the displacement of a more viscous fluid by a less viscous one in a Hele-Shaw cell, as an analogue porous medium, leads to an interfacial instability. This description, however, neglects the inherent disorder in porous media, as well as the non-hydrodynamic interactions between the fluids with the solid surfaces. Here, we revisit the Saffman-Taylor instability using a roughened Hele-Shaw cell and show that the interplay between disorder and wettability of the medium can fundamentally alter the pattern formation dynamics. Our observations show the critical role of the contact-line dynamics in the macroscopic pattern formation, and point to new directions for controlling flows with applications ranging from microfluidics to CO2 sequestration.

References:

Acceptance of Terms and Conditions:

Click here to agree
Poster 4 / 124

When an ink droplet meets coated paper: dynamics

Helder Salvador¹; Herman Wijshoff²; Nicolae Tomozeiu³

¹ Océ Technologies
² Océ Technologies R&D
³ Océ-Technologies B.V.

Corresponding Author(s): nicolae.tomozeiu@oce.com

The physical processes which determine the sessile droplet / porous paper interactions have been the subject of many studies in the last decades. Both theoretical understanding and sustainable industrial applications are the driving forces for these studies. Nowadays, inkjet is one of the main printing technologies, offering the flexibility of digital printing at a breakthrough cost price, productivity, print quality and versatility.

In this work we study the behavior of a sessile droplet on coated media, using experimental setups as high speed camera recordings (HSCR) and Automatic Scanning Absorptometer (ASA) as well as the computational modeling. We aim understanding the three main physical phenomena that dictates droplet dynamics: absorption, evaporation and spreading.

The experimental HSCR data are used to extract the contact angle and base diameter of the droplet, while the ASA data reveal directly the absorption rate of liquids into porous substrates.

To model the evaporation process of water/glycerol mixtures we use the Popov’s theory with Raoul’ts law and activity coefficients. Absorption is modelled using Darcy law with Carman-Kozeny permeability considering the liquid with homogeneous composition. The process of spreading is modelled considering both the pinned and the unpinned droplet on the media. In the first case, the diameter of droplet/substrate interface is constant and the contact angle is determined. For the unpinned case, the Newman formulation is used to determine the contact angle based on the solid-vapor surface tension and the liquid-vapor surface tension, and with this, the base diameter is computed. Surface tension depends on liquid concentration and diffusion/adsorption kinetics of surfactants at the interface.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 5-F / 879

Why different transport behaviors emerge among identical nano- and micro-particles in porous media when repulsion exists

William Johnson¹; Anna RasmusonNone

¹ University of Utah

Corresponding Author(s): william.johnson@utah.edu

A profound change in transport behaviors in porous media occurs for nano- and micro-particles (herein called colloids) in the presence versus absence of repulsion between colloids and collectors (porous media grains). This change is indicated by extended tailing of low colloid concentrations during elution, which is absent or present when repulsion is absent or present, respectively. It also manifests in the spatial distribution of retained colloids with distance from source (herein referred to as retention profiles), which are log-linear when repulsion is absent (favorable attachment conditions) and are either hyper-exponential or non-monotonic when repulsion is present (unfavorable
attachment conditions). The deviation from log-linear retained profiles expected from classic colloidal filtration theory can in some cases transform from hyperexponential to non-monotonic with increased ionic strength, and in some cases non-monotonic profiles may even shift down-gradient with increased elution. These deviations in the presence of repulsion all reflect increased colloid transport distances in the presence versus absence of repulsion that, given the variability of the deviations, are difficult to predict and further confound effective models for water resource protection. Understanding the source(s) of observed deviation from log-linearity is critical for predicting transport distances when repulsion exists, which is expected to be the predominant condition in environmental settings where both colloid and collector surfaces tend to be negatively charged. We herein demonstrate that the apparent distribution of “stickiness” among apparently identical individuals in a colloid population is a natural outcome of physicochemical influences on any colloid population in the presence of colloid-collector repulsion. We demonstrate this using recently-developed representation of the nanoscale charge heterogeneity responsible for colloid attachment in the presence of repulsion combined with trajectory modeling in impinging jet and Happel collectors. Having determined the pore scale origins of deviation from classic colloid filtration theory we upscale these influences to predict transport behaviors successfully at the continuum (column) scale. While field evidence indicates that nanoscale repulsion influences transport at the field scale, we are now in a position to predict and examine the influences of colloid-collector repulsion relative to important field scale effects such as alteration of surfaces via organic and inorganic sorption, precipitation and dissolution equilibria, physical heterogeneity and transient flow.

References:

Acceptance of Terms and Conditions:

Click here to agree

Poster 1 / 962

Why fractures in Marcellus Shale might be plugged too soon: Case study comparing geochemical and geomechanical data obtained from outcrop vs reservoir cores

Hui Du\(^1\); Kristen Carpenter\(^1\); Mileva Radonjic\(^1\)

\(^1\) LSU

Corresponding Author(s): mileva@lsu.edu

Shale rocks play an essential role in petroleum exploration and production because they can occur either as caprocks for subsurface storage in conventional reservoirs or as unconventional reservoir rocks for hydrocarbon extraction via hydraulic fracturing. The ability to produce gas from rocks previously only considered caprocks is an unprecedented and innovative feat, but does not come without an environmental impact and costly issues with permeability reduction of engineered fracture systems. The quantities of water required for hydraulic fracturing and developing these formations for production have been large, and the amounts of flowback and produced water after the hydraulic fracturing processes have been astronomical. These volumes make it imperative that a water recycling solution be found and applied to the development of these fields.

In this study, a batch reaction was conducted with Marcellus shale. Both outcrop and reservoir cores (from different points along wellbore trajectory) were exposed to de-ionized water and a synthetic hydraulic fracturing mixture at reservoir temperature for up to four weeks at a high fluid to rock volume ratio. The chemistry of the created simulated flowback and produced water were analyzed using an ICP. In addition, microstructural analyses were performed in order to establish mineralogical and structural properties, as well as presence of microfractures. Furthermore, indentation tests were conducted at both micro and nanometer level to link the geochemistry and geomechanics of shale rocks, through mechanical properties mapping, the volumetric proportions of each phase can be estimated based on the differential mechanical properties.

The key findings include an analysis of the variation of the simulated flowback water from surface down to cores at a depth of 6420ft, with a focus on heavier mineralogical elements and metals. Less
than 1% of the fluid used in these tests consisted of hydraulic fracturing fluid additives, however, even with this small volume of additives used, a significant difference in mineral dissolution compared to the samples treated with water only was observed. The carbonates in the rock samples showed a high level of dissolution, which can cause an increase in permeability, but can also precipitate causing fracture bridging as well as scale buildup in wellbore structure/pipes. The concentration of Pb was found to be significant in the water comparison, posing a potential environmental issue. The indentation results showed a significant difference in mechanical properties as the result of the alteration in microstructures and mineralogical composition during the batch reaction, and the change of microstructure causing by dissolution/precipitation of individual phase were correlated with the alteration in bulk response of the rock. These findings are preliminary and would require and extensive study that would include numerous samples for different location within Marcellus Shale as well comparison to other producing shale formations.

References:

Acceptance of Terms and Conditions:

Click here to agree

Parallel 2-F / 905

Wicking as partially-saturated flow of a liquid in thin swelling porous media

Ahmed Kaffel\(^1\); Krishna Pillai\(^1\)

\(^1\) University of Wisconsin Milwaukee

Corresponding Author(s): kaffel@vt.edu, krishna@uwm.edu

Unsaturated flow through thin layers of porous media are encountered in many industrial applications, including the liquid-absorbing hygiene products such as wipes, paper towels, and diapers [1-4]. These consumer products demand specific absorbent properties with storage of liquid playing a significant role. Understanding fluid flow and deformation processes in thin swelling porous media is critical for the development and design of these products. We use an averaging approach [5-17] for modeling a system consisting of multiple layers of thin, absorbing swelling porous media as the layer-wise 2D interacting continua, to rigorously derive a 2D averaged macroscopic mass-balance model for each layer and to develop the required constitutive relationships for a system of thin porous layers made of one liquid (water) and two deformable solid phases (fiber and hydrogel). The developed model consists of a set of partial differential equations that keep track the time dependent behavior of variables such as piezometric head, saturation, porosity, and layer thickness, as the liquid moves throughout the multi-layered porous medium. Hence, this model can be used to describe the absorbency process [18], to predict and understand the flow and storage of a liquid in conjunction with the deformation of layers in multilayered thin porous media that is absorbing the liquid, and swelling during deformation. This model will enormously improve the computational speeds, allowing one to develop a fast and reasonably accurate simulation of the unsaturated flow.

The numerical simulations are carried out with the flow parameters and geometries for a few representative cases such as wicking into dry horizontal and inclined porous plates. The simulation predictions, which predict detailed 2-D flow fields, are found to be in good agreement with the experimental and 3D computational results.

References:

18. Feldkamp, J.R., A mathematical description of liquid flow through partially saturated deformable porous media. report 2.02(TL No 7439.).

Acceptance of Terms and Conditions:
Click here to agree

Parallel 1-F / 921

Wicking in the porous pore doublet model

Staffan Lundström

\[1\] Fluid Mechanics, Luleå University of Technology, Sweden

Corresponding Author(s): staffan.lundstrom@ltu.se

The porous pore doublet model that was published in 2008[1] is presented and discussed. The background to the model is that fabrics used for fiber reinforced composite manufacturing often consist of fibers gathered in bundles. Thus, during manufacturing, the liquid resin impregnates a multiscale porous medium and there is a transport between pores of different scales driven by an applied pressure gradient and capillary action. As a simplified version of a fabric a porous pore-doublet model is studied in order to determine the characteristics of the flow. Experiments, as well as theoretical calculations on this generic geometry will be presented.

References:

Acceptance of Terms and Conditions:
Click here to agree

Parallel 2-F / 15

Wind-induced soil-atmosphere gas exchange as related to near-surface wind speed characteristics and soil physical properties

Tjalf Poulsen1; Alireza Pourbakhtiar2

1 Guangdong Technion
2 University of Liverpool

Corresponding Author(s): tjalfe.poulsen@gtiit.edu.cn

Mechanisms of pore gas transport and exchange across the porous medium-atmosphere interface in wind-exposed porous media was investigated for a range of porous media under different near-surface wind conditions. Four dry porous media with mean particle diameters of 1.6, 2.0, 4.2 and 10.5 mm were used. These relatively coarse materials were selected, to facilitate easier identification of the parameters governing wind-induced porous medium gas transport and exchange with the atmosphere. Cylindrical porous medium samples 25 cm in diameter and thickness ranging between 15 and 35 cm were used. Experiments were carried out under controlled conditions for 10 different wind conditions with respect to wind direction, wind speed magnitude and wind speed variability yielding 40 combinations of porous medium and wind condition. Average resultant wind speed as measured 4-12 cm above the porous medium surface ranged between 0.5 and 3 m/s. Tracer (air and CO2) gas breakthrough curves were measured at five depths within each sample. A total of 400 individual tracer gas breakthrough curves (including replicates) were produced. Porous medium gas transport and exchange with the atmosphere was approximated as a one-dimensional dispersive/diffusive process with a depth-dependent dispersion coefficient (Dw). Two models for describing the depth – Dw relationship using two and three empirical fitting parameters, respectively, were evaluated. For each combination of porous medium and wind condition, fitting parameters were determined by numerically solving the dispersion equation (with Dw described by either of the two models), while fitting the solution to all five tracer breakthrough curves simultaneously. In all cases both models yielded close fits to measured breakthrough data. Results showed that in addition to porous medium depth (or distance to the wind-exposed surface), Dw (and thus, gas transport and exchange) was strongly dependent on both mean wind speed, and wind speed power spectrum characteristics, indicating that not only mean wind speed, but also wind gustiness is important. Results further showed that porous medium particle size and to a lesser degree also hydraulic conductivity and air permeability correlated significantly with gas transport and exchange (Dw).

References:

Numerical Design of Porous Materials Using Adjustable Level-Cut Poison Field Method

Author(s): Ben Paisley
Co-author(s): M. Sadegh Riasi; Lilit Yeghiazarian

1 University of Cincinnati

Corresponding Author(s): paislebl@gmail.com

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. Numerical porous media design is one of the possible ways to accelerate this process and to guide manufacturing.

Current numerical porous media design methodologies often include a random microstructure generator nested within an optimization routine. At each iteration, the optimization algorithm compares properties of the microstructure with desired target properties, such as permeability, porosity and pore size distribution, and adjusts 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 at each iteration.

To address this problem, we propose the Adjustable Level-Cut Poison Field (ALCPF) method, a new approach based on the level-cut Poisson field theory [Grigoriu, 2003]. First, several initial domains are generated based on set of filtered Poisson field parameters. Then, rather than generating a completely new filtered Poisson field, the optimization algorithm takes a weighted geometric average of the initial domains to produce a new filtered Poisson field. The process is repeated until an optimal domain is found, with a dramatic reduction in computational time. The weighted geometric averaging also has an added advantage of spatial control over the material microstructure. By adjusting the weights of the geometric mean throughout the initial domains, an inhomogeneous virtual material with desired microstructure can be generated.

References: