Multiphase micro-continuum models: a hybrid-scale approach

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Introduction

- 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 cm², 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-based law in the unresolved (solid-fluid aggregates) regions.
- We extended our micro-continuum model to multiphase flow where surface tension forces between the fluids play an important role in the resolved region.

Imaging and instruments resolution

- Sandstones imaged with a synchrotron facility at 3 μm/voxel have 2% of sub-voxel porosity. We have demonstrated that this sub-voxel porosity was located on the percolation pathways. Assigning fluid or solid phase properties during the image segmentation can lead to an order one error for flow calculations.
- Running flow simulations in shale rock FIB-SEM images is even more complicated: the solid phase properties during the image segmentation can lead to an order one error for flow calculations.
- In the nanoporous region, the Navier-Stokes equation breaks down and molecules are subject to slip effects, Knudsen diffusion, adsorption, surface diffusion.

Micro-continuum model

- Micro-continuum approaches are relevant to model transport in dual-media where only one porosity is resolved.
- The physics in the matrix is described through sub-grid models (ranging from simple Darcy’s law to more complex laws that integrate slip and mesoscale effects).
- For low permeability, low porosity matrix they can be tends to classic pore-scale Navier-Stokes model with immersed boundary condition (relevant for moving boundaries during dissolution for example).

Simulation of methane expulsion in shales

- Scenario A: interfacial phenomena at the surface of hydrophobic wet kerogen limit the recovery of the methane.
- Scenario B (hydrophilic clay in contact with the soaked fracture): Methane is produced as a train of gas bubbles.

Simulation of multiphase dissolution

- The micro-continuum framework with immersed reactive boundary condition is used to simulate calcite dissolution at the pore-scale during the injection of 1% hydrochloric acid in an aqueous solutions, CO₂ gas is produced at the solid surface during the chemical reaction. Gas bubbles, grow, coalesce and detach. The gas recovers part of the solid surface and limit the reaction.
- Simulations compare well with microfluidic experiments.

Under single-phase flow conditions the solid structure dissolves forming wormholes. However, the simulation results for two-phase show that CO₂ bubbles grow, coalesce, and form flow barriers that limit the transport of the acid in the domain. These flow barriers prevent the emergence of wormholes and limit significantly the overall dissolution rate.

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