Pore-scale Modeling and Simulation of flow in Complex Porous Formations

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Outline

Motivations

Digital Rock Physics

A micro-continuum model for flow with reactive surface phenomena

A model for thermal evolution of kerogen-rich shales

A micro-continuum model for multiphase flow

Summary and future steps
Pore-scale processes associated with subsurface CO$_2$ injection and sequestration

1. Drainage, imbibition and trapping mechanism

2. Interphase mass transfer, sCO$_2$/brine dissolution

3. Aqueous speciation, brine pH is lowered, Transport of acid to the mineral surface.

4. Mineral dissolution, wettability alteration

5. Mineral precipitation

Steefel et al., *Pore Scale Processes Associated with Subsurface CO2 Injection and Sequestration* Reviews in Mineralogy and Geochemistry, 2013, 77, 259-303
Thermal evolution of oil-shale

1. Pyrolysis
2. Fluid generation
3. Local pressure increase
4. Fracturing/cracks
5. Liquid/gas transport
6. Production Migration

Allix et al., *Coaxing Oil from Shale* Oilfield Review Winter 2010/2011, 22(4), 4-15
Motivations

Target:

- Understand and model complex physics of flow and transport in reservoirs (conventional reservoir, oil shale retorting, CO2 sequestration, dissolution, ...),
- Replace/complement lab-scale experiments (permeability...)

Challenges:

- Multi-scale problem,
- Multiphase flow,
- Fractured/damaged media,
- Thermal processes,
- Phase change
- Surface chemistry,
- Evolution of the pore structure (dissolution, precipitation, crack propagation...)
- Mechanics,
- ...

CO₂ sequestration into deep saline aquifer and pore-scale CO₂ flow in the native porous media*

Two representations of the physics of fluid

- **direct modeling**
  - "pore-scale"
  - $p_\beta$
  - $\mathbf{v}_\beta$

- **continuum modeling**
  - "Darcy-scale"
  - $\langle p_\beta \rangle^\beta$
  - $\langle \mathbf{v}_\beta \rangle$

for every point of the domain

- fluid **OR** solid
- fluid **AND** solid
Navier-Stokes equations

Mass balance equation
\[ \nabla \cdot \mathbf{v}_\beta = 0 \text{ in } V_\beta, \]

Momentum balance equation
\[ \frac{\partial \rho_\beta \mathbf{v}_\beta}{\partial t} + \nabla \cdot (\rho_\beta \mathbf{v}_\beta \mathbf{v}_\beta) = \begin{cases} -\nabla p_\beta & \text{in } V_\beta, \\ \text{inertia} & \rho_\beta \mathbf{g} & \text{gravity} \\ & \mu_\beta \nabla^2 \mathbf{v}_\beta & \text{viscous term} \end{cases} \]

Non-slip condition at the solid boundary
\[ \mathbf{v}_\beta = 0 \text{ at } A_{\beta\sigma}. \]
Stanford pore-scale modeling activity

- Simulation of flow on real 3D images from micro-CT
- Immiscible two-phase flow
- Multicomponent multiphase mass transfer
- Heat transfer
- Mechanics
- Reactive mass transfer
About the simulation framework

OpenFOAM®

= Open Field Operation and Manipulation

- Solve the Partial Differential Equations using the finite volumes method
- Multiphysic simulation platform mainly devoted to fluid flow
- Manage 3D geometries by default
- Open-source software developed in C++ (object-oriented programming)
- Can be freely download at www.openfoam.org
- Designed as a toolbox easily customisable
- Parallel computation implemented at lowest level
- Cross-platform installation (Linux preferred)

http://web.stanford.edu/~csoulain/OF_Training/
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Summary and future steps
Digital Rock Physics

With the improvement of imaging techniques (micro-CT, synchrotron radiation...) it is now possible to access the exact structure of the solid skeleton...

…and compute the flow in the void space. By volume averaging the resulting velocity profile, we can obtain the permeability tensor.
Digital Rock Physics

- Compute velocity distribution on micro-CT scanned rock samples
- Up to 330 millions cells
- (the maximum sample size depends on the number of pores)
Example: microporosity in a Berea sandstone

Cube 300 x 300 x 300

dark grey: macropores
blue: microporous phase

(Data from P. Gouze, Géosciences Montpellier, France)

3.16 µm = synchrotron resolution

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Micro-continuum approach for pore-scale simulation

Solid and fluid differentiated by the void fraction per control volume:

\[ \varepsilon_f \]

Volume averaged variables:

\[ \bar{v}_f = \frac{1}{V} \int_{V_f} v_f dV \]

\[ \bar{p}_f = \frac{1}{V_f} \int_{V_f} p_f dV \]

The Darcy-Brinkman-Stokes equation allows a single domain formulation

\[ 0 = -\nabla \bar{p}_f + \frac{\mu_f}{\varepsilon_f} \nabla^2 \bar{v}_f - \mu_f k^{-1} \bar{v}_f \]

Vanishes in the void space

Dominant in the porous region

The impact of microporosity on permeability calculation

<table>
<thead>
<tr>
<th>sample</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>K (mD)</td>
<td>518</td>
<td>534</td>
<td>341</td>
</tr>
<tr>
<td>K- (mD)</td>
<td>211 (-59%)</td>
<td>475</td>
<td>305</td>
</tr>
<tr>
<td>K+ (mD)</td>
<td>913</td>
<td>804</td>
<td>673 (+97%)</td>
</tr>
</tbody>
</table>
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Summary and future steps
Modeling of dissolution phenomena

- Develop predictive tools to simulate the evolution of the pore morphology due to reactive transport
- Application to CO₂ sequestration and unconventional
- Application to carbonate acidizing treatments to increase the conductivity near well-bore

Experimental study of fracture evolution due to sCO2 (Courtesy of Jonathan Ajo-Franklin and Marco Voltolini, LBNL)

Experimental study of wormhole formation vs the injection mass flow rate*

Heat and mass transfer with a micro-continuum model

control volume, $V$

Full Navier-Stokes approach

Filtering approach

- All equations are locally averaged,
- Volume fraction of solid is an unknown of the system and evolve with chemistry (ex: dissolution, precipitation, pyrolysis...)
- Flow is governed by Darcy-Brinkman equation

Solid and fluid differentiated by the void fraction per control volume:

$\varepsilon_f$

Volume averaged variables:

$\overline{\mathbf{v}}_f = \frac{1}{V} \int_{V_f} \mathbf{v}_f dV$

$\overline{p}_f = \frac{1}{V_f} \int_{V_f} p_f dV$

Soulaine and Tchelepi Micro-continuum approach for pore-scale simulation of subsurface processes Transport in Porous Media (2016)
Microcontinuum model* for reactive surface

- Darcy-Brinkman model

- Mass balance for solid
  \[ \frac{\partial \varepsilon_s \rho_s}{\partial t} = -\dot{m} \]

- Mass balance for fluid
  \[ \frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla \cdot (\rho_f \bar{v}_f) = \dot{m} \]

- Mass balance equation of acid in the fluid
  \[ \frac{\partial \varepsilon_f \rho_f \bar{\omega}_{f,A}}{\partial t} + \nabla \cdot (\rho_f \bar{v}_f \bar{\omega}_{f,A}) = \nabla \cdot (\varepsilon_f \rho_f D_A^* \nabla \bar{\omega}_{f,A}) - \dot{m}_{f,A} \]

- Rate of dissolution modeled from grain scale
  \[ \dot{m}_{f,A} = \rho_f \alpha^* (\bar{\omega}_{f,A} - \omega_{eq}) \]
  \[ \dot{m} = \Gamma \dot{m}_{f,A} \]


** Soulaine and Tchelepi A micro-continuum approach for pore-scale simulation in subsurface processes Transport in Porous Media (2016)
Pore space evolution with chemistry

2.4mm x 0.7mm

Evolution of the injected concentration

red = high concentration
blue = thermodynamic equilibrium

Simulation

Experiment*

*t = 0
*t = 15 min
*t = 30 min
*t = 45 min

*Song et al., D. Chip-off-the-old-rock: the study of reservoir-relevant geological processes with real-rock micromodels Lab Chip, The Royal Society of Chemistry, 2014, 14, 4382-4390
Simulation of wormholes formation

Grid with 150x150x300 hexahedrals (= 6.75x10^6 cells)**

\[ \varepsilon_0 = 0.1 \pm 3\% \quad \text{and} \quad k_0 = 10^{-11} \text{ m}^2 \pm 10 \% \]

Simulation takes less than 2 hours with 242 cores (Stanford CEES cluster)


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Summary and future steps
CFD model for oil shale pyrolysis

The model is based on a Darcy-Brinkman formulation in a fixed grid that allows the use of the same formulation both in the fractured area and the reactive solid.

$$\frac{\partial \varepsilon_k \rho_k}{\partial t} = -\dot{m},$$

$$\frac{\partial \varepsilon_f \rho_f}{\partial t} + \nabla \cdot (\rho_f \mathbf{u}_f) = \dot{m},$$

$$0 = -\nabla p_f + \mu_f^* \nabla^2 \mathbf{u}_f - \mu_f k_f^{-1} \mathbf{u}_f$$

$$\rho C_p \frac{\partial T}{\partial t} + \rho_f C_{pf} \mathbf{u}_f \cdot \nabla T = \nabla \cdot (\lambda \nabla T) - \Delta H_{pyr} \frac{\partial \rho_k \varepsilon_k}{\partial t}$$

$$\dot{m} = A \exp \left( -\frac{E_a}{RT} \right) \varepsilon_k \rho_k \quad \rho_f = \frac{M_f \rho_f}{RT} \quad k_f^{-1} = k_0^{-1} \frac{(1 - \varepsilon_f)^3}{\varepsilon_f^2}$$

**Soulaine and Tchelepi Micro-continuum approach for pore-scale simulation of subsurface processes Transport in Porous Media (2016)**
Simulation results

Simulation of 1mm x 0.25mm fractured kerogen-rich shales when homogeneously heat up at 570 K during 8 min.

Large excessive pressure in larger grains (related to the distance to the nearest drainage, Kobchenko, 2013) indicates that the grain will crack.

Clearly indicates that a dual continuum model is required at Darcy's scale

*Kobchenko et al., Drainage fracture networks in elastic solids with internal fluid generation, Europhysics Letters (2013)

**Soulaire and Tchelepi Micro-continuum approach for pore-scale simulation of subsurface processes Transport in Porous Media (2016)
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Summary and future steps
Effervescent dissolution

The solid dissolves not only in liquid but also in gas

Formation of droplets of gas

Micro-continuum model for multiphase flow

Volume-of-Fluid (VOF) approach\(^1\)
with CSF\(^2\) and phase change\(^3\)

Evolution of the solid
volume fraction with liquid
acid concentration

Penalized VOF with Darcy
term and wall adhesion
condition (Horgue et al.\(^4\))

Transport of acid concentration with
thermodynamics equilibrium at
gas/liquid interface (Haroun et al.\(^5\))

\(^1\)Hirt, C. & Nichols, B. Volume of fluid (VOF) method for the dynamics of free boundaries Journal of Computational Physics, 1981, 39, 201 - 225
\(^2\)Brackbill et al. A continuum method for modeling surface tension Journal of Computational Physics, 1992, 100, 335 - 354
Effervescent dissolution: simulation results

Contact angle = 45 degrees  
Contact angle = 120 degrees  
Experiments  
(Wen Song and Sophie Roman, SUPRI-A)

Red = solid  
Blue = fluid  
White = gas/liquid interface
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Summary and future steps
Summary and future work

• Start from fundamentals,

• We are building a DNS framework for flow and transport in porous media,

• Pore-scale simulations to get the velocity profile in a pore structure from micro-CT images,

• Unified framework to simulate heat and mass transfer at the pore scale with a micro-continuum approach,

• Extension of the micro-continuum approach to multiphase flow,

• Strong interactions with experimental works (to complement experiments or to validate numerical models).
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• Sophie Roman and Wen Song from SUPRI-A, for providing experimental data for multiphase dissolution,

• Jonathan Ajo-Franklin and Marco Voltolini from LBNL for the dolomite fracture dataset.
Thank you for your attention.

Question?