A level set method for fluid displacement in realistic porous media

Maša Prodanović

Center for Petroleum and Geosystems Engineering
University of Texas at Austin

Department Seminar, Earth Science and Engineering
Imperial College, London
November 4, 2008
Joint work with

Steven Bryant, The University of Texas at Austin

Support

- US Department of Energy, grant "Mechanisms leading to coexistence of gas and hydrates in ocean sediments"
- US Department of Agriculture, grant "Quantifying the mechanisms of pathogen retention in unsaturated soils"

Computational resources

- Texas Advanced Computing Center (TACC)
Outline

- **Introduction**
- **Modeling**
  - Level Set Method
  - PQS Algorithm (Prodanović/Bryant ‘06)
  - Contact angle modeling
  - Coupling with sediment mechanics
- **Results**
  - 2D
  - 3D
  - Coupling with sediment mechanics
- **Conclusions**
Pore scale immiscible fluid displacement

- Fluid-fluid interface (meniscus) at equilibrium with constant capillary pressure $P_c$ and interfacial tension $\sigma$ satisfies Young-Laplace equation

$$P_c = P_{nw} - P_w = \sigma \kappa$$

- We assume quasi-static displacement: at each stage interfaces are constant mean curvature ($\kappa$) surfaces

- Terminology: wetting, non-wetting fluid, drainage, imbibition

\[
\sigma_{AB} \cos \theta = \sigma_{SA} - \sigma_{SB}
\]

Courtesy of D. Wildenschild, Oregon State University
Statement of the problem

- **Goal**
  - **Accurately** model capillarity dominated fluid displacement in porous media

- **What is the big deal?**
  - Calculating constant curvature surfaces
  - Modeling in irregular pore spaces
  - Accounting for the splitting and merging of the interface within the pore space

- **What do we do?**
  - Adapt the **level set method** for quasi-static fluid displacement
Level sets?
Yes, you know about them…

Image courtesy of WWW
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Level set method

- Osher & Sethian, ’88: embed the moving interface as the zero level set of function $\Phi$

- **The evolution PDE:**
  \[
  \phi_t + F |\nabla \phi| = 0, \quad \text{given } \phi(x, 0)
  \]

- $F$ is particle speed in the normal direction, e.g.
  \[
  F'(x, t) = p_c - \sigma \kappa(x, t)
  \]

- **Benefits:**
  - works in any dimension
  - no special treatment needed for topological changes
  - (above F) finding const. curvature surface by solving a PDE
Level Set Method (2)

- Sample speed $F$:
  \[ F(x, t) = p_c - \sigma \kappa(x, t) \]

- Numerical discretization

- Localization, reinitialization

- LSMLIB Level Set Method Library
  - K. T. Chu / M. Prodanović
  - free for research, next release Jan 2009
  - C/C++/Fortran (serial & parallel), Unix-like env.
Progressive quasi-static algorithm (PQS)

- **Drainage**
  - Initialize with a planar front
  - Solve evolution PDE with *slightly compressible curvature model for* $F$ *until steady state:*
    \[ F(\vec{x}, t) = p_c \exp[f(1 - \frac{V(t)}{V_m})] - \sigma \kappa(\vec{x}, t) \]
  - Iterate
    - increment curvature
    - Find steady state of *prescribed curvature model*
      \[ F(x, t) = p_c - \sigma \kappa(x, t) = p_c - \sigma \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \]

- **Imbibition** starts from drainage endpoint and decrements curvature
- Zero contact angle: **wall BC** $\phi = \max(\phi, \psi)$

Porous media geometry

- Described by level set function $\psi$
  - Analytic or real (imaged) input
  - Unaware of individual pores and throats; we can complement network modeling by
    - Computing critical curvatures
    - Stepping in when network not available

Heaviside function

$$H(\psi) = \begin{cases} 
1, & \text{if } \psi \geq 0 \\
0, & \text{if } \psi < 0. 
\end{cases}$$
Geometry: don’t need network modeling, but can help improve it

Model/granular media

Delaunay tesselation → Merging?

Imaged / real media

Segmentation → Medial axis extraction → Throat finding + pore partitioning
Pore-throat network interpretation difficult in multi-scale setting

Image courtesy of Drs. M. Knackstedt & R. Sok, Australian National University
Progressive quasi-static algorithm

non-zero contact angle

- Drainage
  - Initialize with a planar front
  - Solve evolution PDE with slightly compressible curvature model for $F$ until steady state:
    \[ F(\vec{x}, t) = p_c \exp \left[ f \left( 1 - \frac{V(t)}{V_m} \right) \right] - \sigma \kappa(\vec{x}, t) \]
- Iterate
  - Increment curvature
  - Find steady state of prescribed curvature model
    \[ F(x, t) = p_c - \sigma \kappa(x, t) = p_c - \sigma \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|} \]
- Contact angle model
  \[ F(\vec{x}, t) = p_cH(-\psi) - \nabla \cdot (\sigma(\psi) \frac{\nabla \phi}{|\nabla \phi|}) \]

\[ \sigma(\psi) = \begin{cases} 
|\sigma_{SA} - \sigma_{SB}|, & \text{if } \psi \geq 0 \\
\sigma_{AB}, & \text{if } \psi < 0.
\end{cases} \]

\[ \sigma_{AB} \cos \theta = |\sigma_{SA} - \sigma_{SB}| \]
Software available

- LSMLIB Level Set Method Library
  - K. T. Chu / M. Prodanović
  - free for research, next release Jan 2009
  - C/C++/Fortran (serial & parallel), Unix-like env.

- LSMPQS (Progressive Quasi-static alg.)
  - first release planned Feb 2009
Project Objective

*CH₄ hydrates in ocean sediments*

- **Observation**
  - Frequent observation of gas phase coexisting with hydrate phase

- **Objective**
  - Build realistic, grain-scale computational models

- **Hypothesis**
  - Coupled multiphase flow and solid mechanics at the grain scale dictates hydrate growth habit, leading to co-existence of phases

DOE Project ’06, S. Bryant/ R. Juanes
Key phenomena in gas-phase invasion of HSZ occur at **grain-scale**, are coupled.
Coupling with Sediment Mechanics

1. LSM/PQS simulation step @ the given pressure
2. Compute force NW fluid exerts on each grain
3. PFC grain movement due to force exerted by fluid
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2D Fracture ($\theta=0$)

- Drainage (controlled by throats)
- Imbibition (controlled by pores)

Simulation steps (alternating red and green colors). All $\leq 2\%$ rel.abs.err.

Haines jump

Melrose criterion
Curvature – saturation curve

Haines jumps / pore imbibition events $\rightarrow$ saturation jumps
Irreversibility of events $\rightarrow$ hysteresis
2D Throat: $\theta=60$

The last stable meniscus shown in purple: not at geometrical throat!

Simulation, $C=3.88$

Analytic solution, $C=3.89$

Some overlap with solid allowed in order to form contact angle.
2D Fracture: $\theta=30$

- LSMPQS steps shown in alternate red and green colors

Drainage

Imbibition
2D Fracture: $\theta=80$

Drainage

Imbibition: does not imbibe at a positive curvature!

- LSMPQS steps shown in alternate red and green colors
2D Fracture: drainage curves
2D Fracture: imbibition curves

![Graph showing imbibition curves for different contact angles θ.](image)
Fractional wettability: $\theta = 10 \& 80$

Simulation: $C = 4.16$

Analytic solution: 4.23

- Last stable meniscus shown in purple
Mixed wettability: $\theta=60$ & $30$

$C=5.73$
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3D Throat Drainage

- Haines jump in a sphere pack throat, critical curvature close to MSP theory

C=9.0

C=9.1
3D Pore Drainage

C=7.3 and C=7.4  
C=8.4 and C=8.5  
C=12.7 and C=12.8

Haines jumps in adjacent throats followed by drainage of liquid bridges
3D Pore Imbibition

- Melrose criterion @ imbibition observed regardless of the ultimate configuration
- 4 possible critical curvatures,
  \[ C_{i}^{\text{drain}} \geq C_{j}^{\text{drain}} \text{ then } C_{i}^{\text{imb}} \leq C_{j}^{\text{imb}} \]
Sphere Pack - Drainage

A subset from Finney pack of equal spheres
Sphere radius $R=1.0$, discretized at $dx=0.08$ into a $100^3$ sample

PQS drainage simulation endpoint where the non-wetting fluid percolates to the opposite face.
Sphere Pack Drainage (cont’d)

NW phase (left) and W phase (right) at $C=12$, $Sw=0.05$ : W phase in pendular rings around sphere contacts
Sphere Pack Imbibition

capturing snap-off

Capturing snap-off in a throat for two consecutive steps during imbibition

NW phase at C=3.7

NW phase at C=3.6

Zoom: NW phase at C=3.6 with wire-frame surface indicating C=3.7 surface
Comparison to Haines drainage/imbibition experiments in glass bead packing (1930). **Trapped NW phase was not recorded.**
We can easily measure interfacial area, principal and mean curvatures, volumes and number of connected fluid components.
Fractured Berea Sandstone

Fracture image courtesy of Dr. Zuleima Karpyn, PSU

Upscaled fracture 389x116x25
$\Delta x = \Delta y = 0.26 \text{mm}, \Delta z = 0.219 \text{mm}$

$101 \times 25 \times 5.5 \text{mm}^3$
Comparison with Experiment

Aperture field

Experiment, $S_w=0.35$

Simulation $S_w=0.28$

asperities

oil
Fractured Berea Drainage

interface tension oil-water
$\sigma = 41.2 \text{ mN/m}$

$P_2 = 157 \text{ Pa}$  $P_{13} = 607 \text{ Pa}$  W fluid
Fractured Berea Imbibition

- $P_9 = 813$ Pa
- $P_{25} = 153$ Pa
- $P_{26} = 113$ Pa
- $P_{28} = 30$ Pa

Trapped oil

Main oil phase
Fractured Berea Pc-Sw curve
Naturally Fractured Carbonate

- original size $2048^3$
- $dx = 3.1 \mu m$

Image courtesy of Drs. M. Knackstedt & R. Sok, Australian National University
Fractured Carbonate Geometry

Medial surface of 200x230x190 subsample, rainbow coloring indicates distance to the grain (red close, velvet far)
Fractured Carbonate Drainage

Fracture walls impermeable

Non-wetting (left) and wetting phase surface (right) at $C_{16} = 0.11 \mu m^{-1}$
Fractured Carbonate Imbibition

Fracture walls impermeable

Non-wetting fluid (left) and wetting fluid (right) surface, $C_{15} = 0.09 \mu m^{-1}$
Fractured Sphere Pack

*Fracture-matrix transfer*

Pore-grain surface sphere radii $R=1.0$
Image size $160^3$ ($dx=0.1$)

NW phase surface in fracture (drainage beginning)
Fractured Sphere Pack

**Drainage and Imbibition**

Drainage, $C=4.9$

Imbibition, $C=0.24$

Imbibition – rotated, $C=2.15$

Trapped NW phase
Fractured Sphere Pack: C-Sw

In a reservoir simulation fracture+matrix curve might serve as an upscaled input (for a fractured system)
Fracture With Proppant
Towards transfer between two scales

\[ R_1 = 1.0 \]
\[ R_2 = 0.44 \]

Drainage – matrix begun to drain
\[ C = 6.45 \]

C-Sw curve for both drainage and imbibition
Fracture With Proppant

*Residual non-wetting phase*

Residual oil at the imbibition endpoint for two directions of invasion
Throat3D: $\theta=30$

- Throat is bounded by 4 rods in rhomboidal arrangement
- Note: Movie (click button!) shows only non-wet phase surface colored red (meniscus) and gray (solid contact)

C=7.5, last stable main meniscus

C=7.6, only pendular rings remain
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Example sediment: 2D packing of 300 spherical grains

- Micromechanical equations expressed in dimensionless form (and all physical parameters are scaled accordingly)
- Nominal values:
  - Disk Radii: min 0.96, max 2.17, mean 1.35 (µm)
  - Injection pressure: 0.125MPa-0.185MPa
  - Interfacial tension: 0.05N/m

Initialization: Inject gas into 3 selected pores and find the fluid configuration (red) (PQS)

Had grains been unable to move, that would be the end of invasion (packing is tight)
We compute gas configuration and the forces exerted by gas on grains in contact (PQS)

PFC grain-grain contact force network is augmented by gas forces and grains move accordingly

Iterate

Movie:

Fluid pathway opens up between steps 14 and 15
Between steps 18 and 19:
- gas pathway starts branching
- some gas gets trapped by grain movement
Conclusions

- Pore scale fluid displacement modeling via LSM is:
  - Geometrically correct; Haines jumps, Melrose criterion
  - Robust with respect to geometry
  - Modeling (fractional & mixed) wettability possible

- We can easily obtain Pc-Sw curves, fluid configuration details (volumes, areas) – can serve input for upscaled multiphase modeling

- We can observe pore scale phenomena which are overlooked in upscaled simulations
  - The extent to which nonwetting phase is trapped in fracture/enclosed gaps is very sensitive to the direction of the displacement
  - In a reservoir simulation the Pc-Sw curves in matrix+fracture system might serve as an upscaled drainage curve input for a fractured medium.

- Coupling with sediment mechanics!
Thank you!

More Info:
http://www.ices.utexas.edu/~masha

masha@ices.utexas.edu