Lattice Boltzmann simulation of multiphase flow at the pore scale – Implications for improving macroscale flow theories

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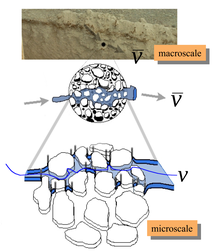
1. Abstract

We review aspects of a new model of multiphase porous media flow. This model is under development and is based on a revised macroscopic theory that more rigorously accounts for the effects of pore-scale interfacial phenomena. A principal feature of this model is its explicit recognition of specific interfacial areas as important macroscopic variables to be incorporated within balance equations and constitutive approximations. A simplified version of the model is presented that allows new parametric data to be studied through experimental, pore-scale flow simulations. Here, we will review how the Lattice Boltzmann method can be used in this effort. We will describe its role and capabilities, as well as some of the application hurdles to be crossed in order to develop new insights into the theory.

2. Macroscopic vs. microscopic vision

- Flow, transport, and reaction processes in porous media
  - Groundwater supply and contamination
  - Petroleum engineering
  - Chemical engineering
- Cannot deal with pore-scale geometry and processes to routinely solve real problems
- Seek to describe processes over appropriate operational scales



3. Flow physics at the macroscopic scale

- Derived from observation, theory, and experiment
- Averaging theory seeks to
  - **Define** macroscopic quantities from volume averages
  - **Integrate** microscale balance laws to macroscopic scale
  - **Approximate** scale transition terms with constitutive models
- Experiments and observations needed to
  - **Validate** constitutive models
  - **Determine** coefficients and other relationships
- Many appropriate macroscopic scales may exist

4. Two-phase flow: Traditional approach

- Simplifications
  - 1D horizontal flow
  - Constant porosity
  - Isothermal
- Basic unknowns:
  - p^w, p^n, s^w, s^n
- Parameters:
  - R^w, R^n
  - permeability, density, viscosity bundled into R terms
- Capillary pressure equation closes system
- Derived as special case of single phase flow. Does that make sense?

Mass and momentum

$$\frac{\partial s^w}{\partial t} - \frac{\partial}{\partial x}\left(\frac{1}{R^w}(s^w)^2\frac{\partial p^w}{\partial x}\right) = 0$$

$$\frac{\partial s^n}{\partial t} - \frac{\partial}{\partial x}\left(\frac{1}{R^n}(s^n)^2\frac{\partial p^n}{\partial x}\right) = 0$$

Geometric constraint

$$s^w + s^n = 1$$

Capillary pressure

$$p^n - p^w = P^c(s^w)$$

Constitutive equations

$$R^w = R^w(s^w)$$
$$R^n = R^n(s^w)$$

5. Paradox A: Equation of State

- May equations of state, typically posed at one scale, be directly applied at another scale?
- At the **microscale**, in a fluid:

  $\rho^w = \rho^w(p^w,T)$, or
  $p^w = p^w(\rho^w,T)$

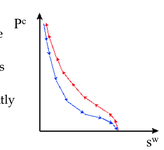
- At the **macroscale**, for the same fluid in a porous medium continuum,

  $p^w = p^n - P^c(s^w) = p^w(s^w)$

- If there is hysteresis in P^c, that is, if there can be different values of P^c for a given value of s^w, or vice versa, depending on the flow history or the path taken, can this truly be an equation of state?
- For multiphase flow in porous media, how should saturation be incorporated into the equations of state?
- Should other variables be incorporated?

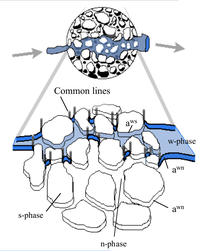
6. Paradox B: Range of values for p^n-p^w =P^c

- The range of reported values for capillary pressure suggests that water pressure must take on large negative values at low saturations.
- Is this realistic or representative of other physics that are not explicitly represented?
- How can these physics be identified and explicitly represented?
- de Marsily observes that P^c measures a state of energy of water in the soil



7. Paradox C: Interfacial effects

- Is the most important difference between saturated and unsaturated flow in the hydraulic conductivity?
- Is a theory that does not formally take into account the evolution and distribution of specific interfacial areas necessarily complete?
- We know that specific interfacial areas
  - Change with saturation
  - Depend on whether drainage or imbibition is in effect
  - Sustain pressure jumps which affect system response to imposed gradients



8. Objectives of this project

- Development of improved theory of macroscopic flow in multiphase systems
  - Focus on effects and impacts of interfacial area
- Development of experimental framework for investigating aspects of the new theory
  - Computational experiments via Lattice Boltzmann simulation
- Construction of new field-scale numerical model based upon new formulation
  - Incorporate simplifications and parametric behavior gleaned from LB simulations

9. Considerations for resolution of paradoxes

- Complete description of system physics requires conservation equations for mass, momentum, energy
- Conservation equations and parameters must be obtained at correct scale of interest
- Conservation equations needed for **phases, interfaces,** and **contact lines**
- Parameters that arise in the formulation must be able to assume physically meaningful values
- Equations and constitutive equations must not violate second law of thermodynamics
- Equations for single phase flow should be obtained as a **special case** from the multiphase formulation, and not the reverse!
- Theoretical results and indications must be confirmed with experimental analyses

10. Approach taken in new equation development

- Derive macroscale conservation equations for phases, **interfaces**, and **common lines**, and the entropy inequality, using volume averaging techniques
- Postulate thermodynamic dependencies of energy on independent variables for phases, interfaces, and common lines, and incorporate within the entropy inequality
- Determine relevant mechanical equilibrium constraints and incorporate within the entropy inequality *(e.g., $\Sigma s^\alpha = 1$, $\delta\varepsilon^\alpha = \ldots$, $\delta\lambda^{\alpha\beta} = \ldots$)*
- Exploit entropy inequality to yield additional constitutive equations that describe system behavior *(e.g., macroscopic form of fluid phase stress tensor)*
- Linearize constitutive functions to obtain closed sets of parameterized equations *(e.g. flow ~ ∇P)*
- Simplify, as appropriate, to forms useful for systems being studied *(e.g., constant T)*
- Seek to interpret physical nature of coefficients, so as to provide insights necessary for design of laboratory experiments *(e.g., k)*

11. Two-phase flow: Revised approach

- Simplifications
  - 1D horizontal flow
  - Constant porosity
  - Isothermal
  - Ignore common lines
  - Dismiss cross-flow interactions
  - Fluid films not handled
- Basic unknowns and parameters
  - p^w, p^n, s^w, s^n
  - R^w, R^n
- New unknowns and parameters
  - a^{wn}, a^{ws}, J^{wn}
  - L_p
- Dynamic capillary pressure
  - Reduces to traditional form at equilibrium

Mass and momentum for w, n phases

$$\frac{\partial s^w}{\partial t} - \frac{\partial}{\partial x}\left(\frac{1}{R^w}(s^w)^2\frac{\partial p^w}{\partial x}\right) = 0$$

$$\frac{\partial s^n}{\partial t} - \frac{\partial}{\partial x}\left(\frac{1}{R^n}(s^n)^2\frac{\partial p^n}{\partial x}\right) = 0$$

Geometric constraint

$$s^w + s^n = 1$$

Dynamic capillary pressure

$$L_p\frac{\partial s^w}{\partial t} = -\left[p^n - p^w + \sigma^{wn}J^{wn}\left(s^w, a^{wn}, a^{ws}\right)\right]$$

Constitutive equations for $R^{w,n}$

$$R^w = R^w(s^w, a^{wn}, a^{ws})$$
$$R^n = R^n(s^w, a^{wn}, a^{ws})$$

12. Dynamic capillary pressure: three important implications

- At equilibrium, the "traditional" capillary pressure is balanced exactly by the product of mean curvature and interfacial tension. Since the mean curvature is postulated to be a function of both saturation and the mean interfacial areas per unit volume, the usual assumption that capillary pressure (at equilibrium) is only dependent on saturation would appear to be incomplete.
- Away from equilibrium, under transient, flowing conditions, there appears to be a dynamic "capillary pressure" that differs from the mean curvature by the term proportional to the rate of change of saturation. Thus, dynamic and equilibrium conditions need to be separately accounted for in models and experimental measurements. Kalaydjian [1992] proposed a similar result.
- Additional geometric balance equations for the interfacial areas are now required for closure purposes.

13. Additional closure equations

- Mean curvature (J^{wn}) postulated to be dynamic function of saturation and interfacial area
- Changes in a^{ws} related to unbalanced forces where interfaces intersect surface
  - Equilibrium implies balanced forces on common lines
  - L_{ws} ~ parameter
- Changes in a^{wn} related to changes in s^w, a^{ws}, and interfacial velocity (v^{wn})
  - G^{wn} ~ shape factor
  - Equilibrium implies constant value of $G^{wn}a^{wn}v^{wn}$

Mean w-n curvature

$$J^{wn} = J^{wn}(s^w, a^{wn}, a^{ws})$$

w-s interfacial area

$$L_{ws}\frac{\partial a^{ws}}{\partial t} = -(\sigma^{ws} - \sigma^{ns} + \sigma^{n}\cos\Phi^{w})$$

w-n interfacial area

$$\frac{\partial a^{wn}}{\partial t} - \varepsilon J^{wn}\frac{\partial s^w}{\partial t} - \cos\Phi^{w}\frac{\partial a^{ws}}{\partial t} = -\frac{\partial}{\partial x}\left(G^{wn}a^{wn}v^{wn}\right)$$

w-n interfacial area velocity

$$v^{wn} = R_1 v^w + R_2 v^s$$

Mean solid-interface contact angle

$$\Phi \sim \Phi\left(s^w, a^{wn}, a^{ws}\right)$$

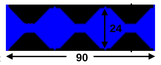
14. Further insight requires experimentation

- Consider **dynamic capillary pressure equation:**
- Understanding and ultimate application requires
  - Measurement of coefficient L_p
  - Measurement of interfacial area and saturation
  - Measurement of J^{wn} and its dependence on interfacial area and saturation
- Can this be done? How?
  - Dynamic coefficient L_p has been measured in physical column experiments (Kalaydjian, 1992)
  - Equilibrium configuration of interfacial areas has been measured in a crushed glass porous medium (Montemagno and Gray, 1996)
  - Equilibrium J^{wn} "surface" has been measured from a capillary network model (Reeves and Celia, 1996)
- Can dynamic simulations provide any further insight?
  - Explore use of Lattice Boltzmann simulations

15 Lattice Boltzmann "basics" on separate sub-poster!

16. Simple example: Effect of wettability on interfacial area

- Defined a simple domain
  - 3-D Sinusoidal tube:
- Modify solid surface wettability:
  - Strongly water (blue) wet
  - Mildly water wet
  - Strongly oil (red) wet
  - Wetted by neither
  - Upper half (z > 0) water wet, lower half oil wet
  - Bands of alternating water wet and oil wet, (20 units) in x dir.
- Run pressure driven displacement problem
  - Water (w) displaced by oil (n)
  - Measure sw, p^w, p^n , a^{wn}, a^{ws} as f(time)
  - Apply measured values to theory

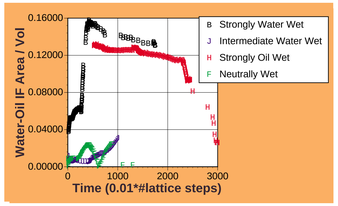


17. What is wettability?

- **Wettability:** The dominance of molecular attraction between the surface and one of the liquids over the other or the cohesive force of the liquid itself.
  - Depends on the fluids AND the solid
  - Typically quantified by equating it with the contact angle of the fluid with the solid:
- Why is it important?
  - Affects the regions occupied by a fluid and the behavior of fluids in a porous medium
  - Changes the relative permeability response

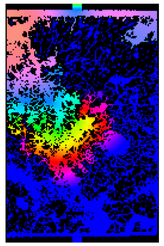
19. Interfacial area versus time as function of solid surface wettability (Φ)

- Sinusoidal tube "experiments"
  - Wettability strongly affects area vs time behavior



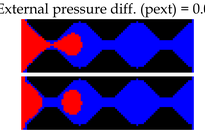
20. Summary and the future

- Multiphase flows in porous media are extremely complicated
- Theoretical work is leading to better understanding of the fundamental physics involved
  - Systematic incorporation of surface areas as important variables
  - Dynamic nature of capillary pressure
- Lattice Boltzmann simulation of pore scale flow offers a particular approach for experimental investigations
- LB simulations still underwu
- R&D Transition based upon
  - Development of field simulator
  - Field methods to measure interfacial area (e.g., Saripalli, et al. 1996)
- Future applications can be directed at improving theories of macroscopic transport and reaction in porous media

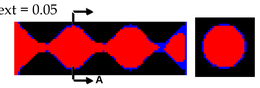


18a. Strongly water wetted walls

- External pressure diff. (pext) = 0.01



- Pext = 0.05

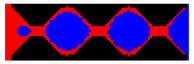


- Pext = 0.075

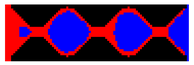
Water Oil Solid

18b. Strongly oil wetted walls

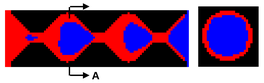
- Pext = 0.01



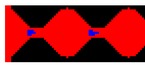
- Pext = 0.05



- Pext = 0.075

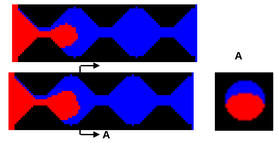


- Pext = 0.1



18c. Mixed Wettability Walls

- Top is Strongly Water Wet
- Bottom is Strongly Oil Wet
- Pext = 0.01, t = 10k, 100k



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Some basics of Lattice Boltzmann simulation methods

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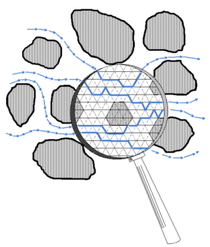
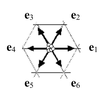
15a. Lattice gas/Lattice Boltzmann models

- Fluid represented by discrete particles
- Advection and collision on regular lattice
- Ensemble behavior reproduce Navier Stokes behavior
- Advantages
  - Simple computational operations
  - Fast, naturally parallel
  - Stable
  - Conserves mass, momentum,



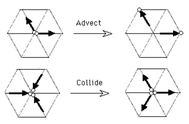
15b. Lattice gas model: 2-D example

- Lattice
  - hexagonal with 6 link directions $\mathbf{e}_i$
- Particles
  - Unit mass
  - Discrete velocity, $\mathbf{e}_i$
  - Boolean existence, $n_i(\mathbf{r},t) = 0$ or 1
  - Statistical average, $\langle n_i(\mathbf{r},t) \rangle = N_i(\mathbf{r},t)$
- Mass density
  - $\rho(\mathbf{r},t) = \Sigma_i\, n_i(\mathbf{r},t) \rightarrow \Sigma_i\, N_i(\mathbf{r},t)$
- Momentum density
  - $\rho\mathbf{v}(\mathbf{r},t) = \Sigma_i\, \mathbf{e}_i\, n_i(\mathbf{r},t) \rightarrow \Sigma_i\, \mathbf{e}_i\, N_i(\mathbf{r},t)$
- Momentum flux
  - $\Pi(\mathbf{r},t) = \Sigma_i\, \mathbf{e}_i\, \mathbf{e}_i\, n_i(\mathbf{r},t) \rightarrow \Sigma_i\, \mathbf{e}_i\, \mathbf{e}_i\, N_i(\mathbf{r},t)$



15c. Lattice gas model: One time step

- Particles **advect** along lattice links
- Particles **collide** and **redistribute** velocities
- Collision rules
  - Conserve mass and momentum
  - Change nonequilibrium (viscous) part of momentum flux
  - 2^6 possible collisions for this lattice
- Continuum fluid physics affected by
  - Flexibility in collision rules
  - Lattice configuration
  - Number of particles allowed



15d. Lattice gas model: Continuum limit

- Ensemble population follows Fermi-Dirac distribution: $N_i = (1 + \exp(\alpha(\rho,u)+\beta(\rho,u)\,\mathbf{e}_i\cdot\mathbf{v}))^{-1}$
  - When $\mathbf{v} = 0$, $\rho = N_i / 6$
  - Taylor expansions of α and β around $\mathbf{v} = 0$ leads to

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) = 0$$

$$\frac{\partial\rho\mathbf{v}}{\partial t} + \nabla\cdot(\rho g(\rho)\mathbf{v}\mathbf{v}) = -\nabla P - \mu\nabla^2\mathbf{v}$$

$$P = \rho c_s^2 = \rho/2$$

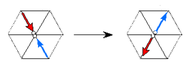
- Under some conditions, rescaling
  - restores incompressibility (low Mach number)
  - Gallilean invariance
  - Body force (gravity)
- Lattice Boltzmann approach
  - Update N_i directly
  - Built on discrete analog of Boltzmann equation
  - More flexible

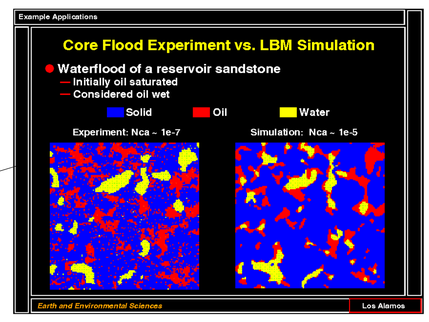
15e. Lattice gas vs. Lattice Boltzmann

Calculate:	**Actual** particle occupation	**Expected** particle occupation
	$n_i(\mathbf{r}+\mathbf{e}_i,t+1) = n_i(\mathbf{r},t) + \Omega_i$	$N_i(\mathbf{r}+\mathbf{e}_i,t+1) = N_i(\mathbf{r},t) + \Delta_i$
Arithmetic:	Integer, bit (0 or 1)	Real, floating point (0 – 1)
Stability:	Unconditional	Conditional
Equilibrium:	Function of collisions	Specified directly
EOS:	Velocity dependent	Ideal gas
Invariance:	non Galilean effect	Invariant
3D:	4D FCHC lattice	3D BCC lattice
Results:	"spatially noisy"	spatially smooth

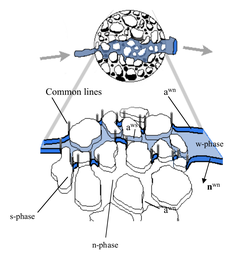
15f. Two-phase Lattice Boltzmann flow

- Particles come in two "colors"
- Collision function biases particles to stay with like colors
  - Conserve mass of each color
  - Conserve momentum of both colors together
  - Minimize energy of collision
  - Minimize flux of color
- Surface features (wettability) can be specified
- Dynamic behavior easily observed
- Reproduces
  - Known equilibrium surface tension effects (Laplace curvature, etc.)
  - measured permeabilities
  - Core flood saturation profiles





15g. Dynamic numerical experiments via LB

- Ideal procedure
  - Run dynamic flow experiments in discrete 3D porous geometries
  - Interrogate solutions over time to measure averaged quantities
  - Reconcile with theory
- Easy part
  - Fluid saturations
  - Macroscopic phase velocities and pressures
  - Interfacial areas
- Hard part
  - Mean curvature
  - Mean interfacial velocities
- Recognize potential limitations
  - Limited physics (e.g., no film flow)
  - Compute intensive, tons of data

$$J^{wn} \sim \frac{1}{A^{wn}} \int_{A^{wn}} \nabla\cdot\mathbf{n}^{wn}\, da$$