Two-phase flow relative permeability determination using lattice Boltzmann method at the pore scale

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The context: two-phase flow modeling in radioactive waste disposal
Two-phase flow modeling at the radioactive waste repository scale.

- Anaerobic corrosion of metallic objects introduced inside the radioactive waste repository (canisters) is expected to produce a significant amount of hydrogen.

- The impact on repository behavior must be quantified:
  - Early gas breakthrough ($^{14}$C)?
  - Degradation of components confinement properties (pressure build-up)?
  - Host-rock fracking?
  - Plugs and sealing / host-rock interface degradation (by-pass)?
Two-phase flow modeling at the radioactive waste repository scale.

- Part of quantification is made through computation

Two-phase flow (mass balance)

\[
\theta \frac{\partial}{\partial t} S_{e, w} - \nabla \left( \frac{k_{\text{int}} k_w}{\eta_w} \nabla (p_w + \rho_w g z) \right) = Q_w
\]

\[
\theta \frac{\partial}{\partial t} S_{e, mw} - \nabla \left( \frac{k_{\text{int}} k_{mw}}{\eta_{mw}} \nabla (p_{mw} + \rho_{mw} g z) \right) = Q_{mw}
\]

FORGE results
Two-phase flow modeling at the radioactive waste repository scale.

- Relative permeability ($Kr(S)$) has a strong impact on the results but is not well known.

\[
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\]

\[
\theta \frac{\partial}{\partial t} S_{e,mw} - \nabla \left( \frac{k_{mw}}{\eta_{mw}} \nabla (p_{mw} + \rho_{mw} g z) \right) = Q_{mw}
\]

- Determination of $Kr$ through experimental measurements is very difficult in argillaceous rocks because of their very small permeability (PhD. Yang 2008).
  - Indirect determination through capillary curve and Mualem theory.
Two-phase flow modeling at the pore scale.

- We decided to quantify $K_r(S)$ through pore scale modeling → like for permeability, effective diffusion …

- What is the pore scale to consider? → Small fractures of few microns in thickness are of major concern for two-phase flow (gas do not enter smallest pores).

- What is the best numerical approach? → Lattice Boltzmann methods were extensively used for pore scale modeling purpose.
The context: two-phase flow modeling inside radioactive waste disposal

- Lattice Boltzmann approach

- Application: two-phase flow at the pore scale
The lattice Boltzmann approach.

Lattice Boltzmann approach originates from cellular automaton approach that mimic fluid behavior through “particles” propagation and collision.

In the lattice Boltzmann approach, mass, time and space are discretized. Space is discretized using a regular grid and velocity space is discretized in Q directions.

A “population function” $f$ is associated to each node $x$ for each direction $q$ that evolves through a “collision step” and a “propagation step”.
The lattice Boltzmann approach.

“Collision step”

\[ f_q(x,t+dt) = f_q(x,t) + (f_q^{eq} - f_q(x,t))/\tau \]

“Propagation step”

\[ f_q(x+e_i,t+dt) = f_q(x,t+dt) \]

Modeled physic depend on the choice of \( f_q^{eq} \)
(for fluid flow \( \rho = \sum f_q \) and \( \rho u = \sum f_q e_i \))

\( \tau \) is a relaxation time parameter (BGK, TRT, MRT)

Note that equivalence of LBM scheme and finite difference Du Fort-Frankel scheme was shown for 1D heat transfer equation (Dellacherie, *Acta Applicandae Mathematicae*, 2014)
Lattice Boltzmann model

- Lattice Boltzmann models used to simulate two-phase flow are very numerous.

- Among the LBM zoology we use the two color RK model (color gradient model, Rothman & Keller 1988) with a Two Relaxation Time scheme (TRT) (Ginzburg et al. 2008)
  
  → one collision step
  
  → one re-coloration step
  
  → one propagation step
Lattice Boltzmann model

RK model in detail

Collision

$$\Omega^1(f_q) = f_q + \lambda_{even}(f_q^+ - f_q^{eq. +}) + \lambda_{odd}(f_q^- - f_q^{eq. -}) + S_q$$

Perturbation – Recoloring

$$\Omega^2(f_q) = f_q + \frac{A_{r,b}}{2} \nabla \cdot \vec{c} \left( \frac{(\nabla \cdot \vec{c})^2}{||\nabla \cdot \vec{c}||^2} - B_q \right)$$

$$\Omega^3(f_q) = \beta \frac{\rho_r \rho_b}{\rho^2} \cos(\theta_q) f_q^{eq}|_{\nabla = 0}$$

$$r_q = \frac{\rho_r}{\rho} \Omega^2(f_q) + \Omega^3(f_q), \quad b_q = \frac{\rho_b}{\rho} \Omega^2(f_q) + \Omega^3(f_q)$$

Propagation

$$f_q^{temp} = r_q + b_q, \quad f_q(\vec{v} + \vec{c}_q, t + \Delta t) = f_q^{temp}(\vec{v}, t)$$

Bounceback

When the q direction neighbor is a solid site, the distribution is "bounced back" in the q direction,

$$f_q(\vec{v} + \vec{c}_q, t + \Delta t) = f_q^{temp}(\vec{v}, t)$$

- $f_q^-, f_q^+$ : odd and even parts of the distributions
- $\lambda_{even}, \lambda_{odd}$ : TRT relaxation parameters
- $S_q$ : source term

- $r, b, \rho_r, \rho_b$ designate the two phase distributions and densities
- $\nabla \cdot \vec{c}$ : Color or phase gradient
- $\beta, A_{r,b}$ : Interface parameters
- $\theta_q$ : angle formed by $(\nabla \cdot \vec{c}, \vec{c}_q)$

- Propagation is done in a second temporary array $f^{temp}$

- $q$ and $\vec{v}$ are velocity opposite directions
Lattice Boltzmann model advantages and drawbacks

- **Advantages**

  Porous geometries like the ones obtained through computed tomography (voxels) are naturally integrated (LBM node). → No meshing work needed.

  Structure of the LBM (node by node description with no matrix inversion) allow efficient parallelism implementation.

- **Drawback**

  Computations are conducted using “LBM fluids parameters” which are “different” from the fluids physical parameters (density, viscosity). → dimensional scaling is mandatory.
Dimensional analysis

- Two phase flow physics in porous media is defined through 4 dimensional numbers Re, M, Ca, Bo

- \( L = 10^{-6} \text{ m} \); \( V = 10^{-7} \text{ m/s} \)

- \( \text{Re} = \frac{\rho_w V L}{\mu_w} = 1000 \times 10^{-7} \times 2 \times 10^{-6} / 10^{-3} = 2 \times 10^{-7} \)

- \( \text{M} = \frac{\mu_w}{\mu_g} = 10^{-3} / 10^{-5} = 100 \)

- \( \text{Ca} = \frac{\mu_w V}{\sigma} = 10^{-3} \times 10^{-7} / 75 \times 10^{-3} = 1.3 \times 10^{-10} \)

- \( \text{Bo} = \frac{\Delta \rho g L^2}{\sigma} = 1000 \times 10 \times (2 \times 10^{-6})^2 / 75 \times 10^{-3} = 5 \times 10^{-7} \)
Cuda (*Compute Unified Device Architecture*)

- CPU use GPU as a set of multi-processors units:
  - NVS 5200M: 2 x 48 = 96
  - Tesla C2050: 14 x 32 = 448

- ++++ Equivalent to parallelism.
- Slight programming changes → sequential functions
- Small memory for elementary operation
- Don’t like conditional operation
The context: two-phase flow modeling inside radioactive waste disposal

Lattice Boltzmann approach

Application: two-phase flow at the pore scale
Two-phase flow at the pore scale: preliminary computations

- Free numerical parameters of the model were adjusted in order to fit the relevant dimensional numbers describing two-phase flow in fractures when gravity effects are neglected (capillary number, mobility ratio).

  LBM parameters \rightarrow LBM fluids properties \rightarrow Ca, M

- The resulting RK model was tested against analytical solutions for static (Laplace law) and dynamic (Poiseuille flow) conditions.
Two-phase flow at the pore scale: static test

We tested our LBM against the Laplace law and verified that the pressure difference in fluids $\Delta P$ for a bubble is linearly dependent in $2\sigma/R$ (with $\sigma$ the surface tension and $R$ the radius of the bubble).
Two-phase flow at the pore scale: dynamic test

We tested our LBM against the Poiseuille flow analytical solution (2 fluids / 3 layers) and verified that the velocity profile match the analytical one for our viscosity ratio.

Rannou, 2008
We tested our LBM against the Poiseuille flow analytical solution (2 fluids / 3 layers) and verified that the velocity profile match the analytical one for our viscosity ratio.
Two-phase flow at the pore scale: dynamic test

- Bubble flow (Channel = 32x32x120 sites; Bubble diameter = 24 sites)
Two-phase flow at the pore scale

Two-phase flow in fracture (system = 40x400x400)
Two-phase flow at the pore scale: Kr computation

- Two-phase flow in fracture

\[ V_{\text{sat}} = -K_i \text{grad } H \]
\[ V_S = -K_i \text{Kr}(S) \text{grad } H \]

\[ \rightarrow \text{Kr}(S) = \frac{V_S}{V_{\text{sat}}} \]
Rothman and Keller LBM (TRT) was selected and implemented on GPU using CUDA (x64 performance // CPU)

Verification tests were successfully performed on static and dynamic problems with analytic solutions.

First two-phase flow computations in argillite micro-fractures are promising.