Modeling Multiphase Flow in Porous Media

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Applications of Multiphase Flow

- Carbon sequestration
- Groundwater management
- Contaminant transport
- Oil and gas recovery


Overall Goals

- Implement the nonlinear complimentarity constraints approach to solve a system of PDEs and constraint equations modeling multiphase flow in Amanzi.
- Provide a capability to model fully coupled 2-phase, 2-component, non-isothermal, miscible flow with phase transitions.
- Develop unit tests for verification.
- Pursue application to realistic problem such as desiccation.
Phase I

- Develop confidence working with Amanzi.
- Formulate a coupled system of pressure and saturation equations.
- Implement a fully implicit approach to solve this system of equations.
- Develop unit tests for pressure and saturation equations.
System of Equations

\[
\begin{align*}
\frac{\partial}{\partial t} \left( \phi \sum_{\alpha=w,n} \rho_{mol,\alpha} X^K_{\alpha} S_{\alpha} \right) + \nabla \cdot \left( - \sum_{\alpha=w,n} \left( \rho_{mol,\alpha} X^K_{\alpha} v_{\alpha} + D^K_{pm,\alpha} \rho_{mol,\alpha} \nabla X^K_{\alpha} \right) \right) &= f^K \\
\frac{\partial}{\partial t} \left( \phi \sum_{\alpha=l,g} \rho_{mass,\alpha} u_{\alpha} S_{\alpha} + (1 - \phi) \rho_s c_s T \right) + \nabla \cdot \left( - \sum_{\alpha=1}^M \left( \rho_{mass,\alpha} h^K_{\alpha} v_{\alpha} \right) + \sum_{K=1}^N \sum_{\alpha=w,n} \left( D^K_{pm,\alpha} \rho_{mol,\alpha} h^K_{\alpha} M^K \nabla X^K_{\alpha} \right) - \lambda_{pm} \nabla T \right) &= f^h \\
v_{\alpha} &= \frac{\kappa_{r\alpha}}{\mu_{\alpha}} K \left( \nabla p_{\alpha} - \rho_{mass,\alpha} g \right) \\
p_c(S_I) &= p_n - p_w, \\
S_w + S_n &= 1, \quad 0 \leq S_{\alpha} \leq 1, \quad \sum_{K=1}^N X^K_{\alpha} = 1, \quad 0 \leq X^K_{\alpha} \leq 1
\end{align*}
\]
We made the following simplification

- Immiscibility, no phase transition.
  - No molar fractions.
  - No additional constraints for local thermal dynamic equilibrium.

- Isothermal
  - No energy equation.
  - Densities, porosity, and viscosities independent of temperature.

- Incompressibility
  - The fluid and solid structure (rock matrix) is incompressible.
  - Densities and porosity constant in space and time.
For phase $\alpha$, we have

$$
\frac{\partial (\phi \rho_\alpha S_\alpha)}{\partial t} + \nabla \cdot \left( \rho_\alpha v_\alpha \right) = q_\alpha, \quad \alpha = w, n
$$

(1)

in which

- $\phi$ is the porosity
- $\rho_\alpha$ is the density of phase $\alpha$
- $S_\alpha$ is the saturation of phase $\alpha$
- $v_\alpha$ is the Darcy’s velocity of phase $\alpha$
- $q_\alpha$ is the source term of phase $\alpha$.

In addition, we have the constraint

$$
\sum_\alpha S_\alpha = 1
$$

(2)
Constitutive Relations

We use extended Darcy’s law for multiphase flow

\[ \mathbf{v}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} K (\nabla P_\alpha - \rho_\alpha \mathbf{g}), \quad \alpha = w, n \]  

(3)

where
- \( K \) is the absolute permeability
- \( k_{r\alpha} \) is the relative permeability of phase \( \alpha \)
- \( \mu_\alpha \) is the viscosity of phase \( \alpha \)
- \( P_\alpha \) is the pressure of phase \( \alpha \)
- \( \mathbf{g} \) is gravity

The phase pressures are related through capillary pressure \( P_c \)

\[ P_c = P_n - P_w \]  

(4)
Relative Permeability

Common models for relative permeability $k_{r\alpha}$

- **Power law (Brooks-Corey type)**

  \[ S_{e\alpha} = \frac{S_{\alpha} - S_{r\alpha}}{1 - \sum_{\beta} S_{r\beta}} \]  
  \[ k_{r\alpha} = (S_{e\alpha})^n \]  

- **Van Genuchten [Genuchten, 1980]**

  \[ k_{rw}(S_w) = \sqrt{S_{ew}} \left( 1 - \left( 1 - S_{ew}^{1/m} \right)^m \right)^2 \]  
  \[ k_{rn}(S_w) = \sqrt{1 - S_{ew}} \left( 1 - S_{ew}^{1/m} \right)^{2m} \]
Models for capillary pressure $P_c$

- **Brooks-Corey** [Brooks and Corey, 1964]

  $P_c(S_w) = P_d S_w^{−1/λ} \quad (9)$

- **Van Genuchten** [Genuchten, 1980]

  $P_c(S_w) = P_r \left( S_{e_w}^{−1/m} − 1 \right)^{1/n} \quad (10)$

  $m = 1 − 1/n \quad (11)$
Pressure Equation

Sum the mass balance equations, with $\sum_{\alpha} S_{\alpha} = 1$,

$$\nabla \cdot \left( \sum_{\alpha} \frac{k_{r\alpha}}{\mu_{\alpha}} \rho_{\alpha} v_{\alpha} \right) = \sum_{\alpha} \frac{q_{\alpha}}{\rho_{\alpha}}$$

(12)

In short form

$$\nabla \cdot v = q$$

(13)

where $v = v_w + v_n$ is the total velocity and $q$ is the total source term.

$$v = -\left( K\lambda_w (\nabla P_w - \rho_w g) + K\lambda_n (\nabla P_n - \rho_n g) \right)$$

(14)

$$q = \frac{q_w}{\rho_w} + \frac{q_n}{\rho_n}, \quad \lambda_w = \frac{k_{rw}}{\mu_w}, \quad \lambda_n = \frac{k_{rn}}{\mu_n}$$

(15)
Introducing fractional flow of the wetting phase $f_w$, with total mobility

$$\lambda = \lambda_w + \lambda_n$$

$$f_w = \frac{\lambda_w}{\lambda} \quad (16)$$

Total velocity becomes

$$v = \lambda K (\nabla P_n - f_w \nabla P_c - G) \quad (17)$$

$$G = \frac{\lambda_w \rho_w + \lambda_n \rho_n}{\lambda} g \quad (18)$$

Define global pressure such that

$$\nabla P = \nabla P_n - f_w \nabla P_c \quad (19)$$
Fractional Flow (cont.)

One common choice for global pressure $P$ [Chavent and Jaffré, 1978] is

$$P = P_n - \pi(S_w)$$  \hspace{1cm} (20)

$$\pi(S_w) = \int_{S_0}^{S_w} f_w(\xi) \frac{\partial P_c}{\partial S_w}(\xi) d\xi + \pi_0$$  \hspace{1cm} (21)

Then the total velocity is reduced to

$$\mathbf{v} = \lambda K (\nabla P - \mathbf{G})$$  \hspace{1cm} (22)

The pressure equation only depends on the global pressure $P$

$$-\nabla \cdot \left( \lambda K (\nabla P - \mathbf{G}) \right) = q$$  \hspace{1cm} (23)

$\Rightarrow$ Diffusion equation
Saturation Equation

Using the mass balance equation for the wetting phase,

\[
\phi \frac{\partial S_w}{\partial t} + \nabla \cdot \mathbf{v}_w = \frac{q_w}{\rho_w} \quad (24)
\]

Rewrite the Darcy’s velocity of the wetting phase \( \mathbf{v}_w \) using total velocity \( \mathbf{v} \) and fractional flow \( f_w \)

\[
\mathbf{v}_w = f_w \mathbf{v} + \lambda_n f_w K (\nabla P_c + (\rho_w - \rho_n) \mathbf{g}) \quad (25)
\]

⇒ Nonlinear advection equation
Approach

We have a coupled system of

- Pressure equation: linear elliptic PDE.
- Saturation equation: nonlinear scalar hyperbolic PDE.

Common approach

- Implicit pressure explicit saturation (IMPES) in which the saturation equation is solved explicitly.
- Semi-implicit schemes.
- **Fully implicit approach in which the saturation is solved implicitly. (Our project)**

For simulation, we solve pressure and saturation equations sequentially in that order, with some initial condition for saturation.
We use finite volume method in space

\[ - \sum_{j \in \eta_i} \int_{\gamma_{ij}} \lambda K \nabla P \cdot n dS = V_i q \]  \hspace{1cm} (26)

On each face, the pressure gradient is approximated with two point flux approximation (TPFA)

\[ - \int_{\gamma_{ij}} \lambda K \nabla P \cdot n dS = -|\gamma_{ij}| \frac{2(P_i - P_j)}{\Delta x_i + \Delta x_j} (\lambda K)_{ij} \]  \hspace{1cm} (27)

We compute the transmissibility using harmonic average.

\[ (\lambda K)_{ij} = (\Delta x_i + \Delta x_j) \left( \frac{(\lambda K)_i (\lambda K)_j}{\Delta x_i (\lambda K)_j + \Delta x_j (\lambda K)_i} \right) \]  \hspace{1cm} (28)
We use finite volume in space and backward Euler in time. For each control volume,

\[ V \phi \frac{S_{w}^{n+1} - S_{w}^{n}}{\Delta t} + \int_{\partial V} f_{w}(S_{w}^{m}) \mathbf{v} \cdot \mathbf{n} = V \frac{q_{w}^{m}}{\rho_{w}} \]

In IMPES approach, \( m = n \), and for fully implicit approach, \( m = n + 1 \).

The fractional flow is upwinded

\[ f_{w}(S_{w})_{ij} = \begin{cases} f_{w}(S_{w})_{i} & \text{if } v_{ij} \cdot \mathbf{n} \geq 0 \\ f_{w}(S_{w})_{j} & \text{if } v_{ij} \cdot \mathbf{n} < 0 \end{cases} \]

The total velocity \( \mathbf{v} \) is calculated from the solution of the pressure equation.
Amanzi: The ASCEM Multi-Process HPC Simulator

- Modular HPC simulation capability for waste form degradation, multiphase flow and reactive transport.
- Efficient, robust simulation from supercomputers to laptops.
- Design and build for emerging multi-core and accelerator-based systems.
- Open-source project with strong community engagement.

Wide Range of Complexity

Wide Range of Platforms
Amanzi: Approach and Features

- **Structured / Unstructured mesh capability:**
  - Leverages mesh frameworks (MSTK, STKmesh) for general unstructured meshes.
  - Leverages structured AMR techniques and libraries (BoxLib)

- Leverages the Trilinos framework (Epetra, Thyra) and supporting tools/solvers.

- Leverages advances in Mimetic Finite Difference (MFD) methods to enable accurate solutions.
  - mixed-hybrid (or local) formulation
  - arbitrary polyhedra (layered media, pinch-outs)
  - distorted meshes (capture topography and hydrostratigraphy)
  - discontinuous and highly variable anisotropic coefficients (permeability)
Amanzi Design

Components of Amanzi. [Coon et al., 2014]

Goal: Ensure domain scientists can easily understand, extend, and develop PK implementations.
Arctic thermal-hydrology model:

- Thermal hydrology with surface and subsurface flow is strongly coupled.
- This MPC is weakly coupled to the surface energy balance.
- The hierarchical use of MPCs makes these coupling scenarios easy to express.

An example of a process kernel tree for a model of thermal hydrology in the arctic. [Coon et al., 2014]
What have we accomplished?

For phase I, we have implemented in Amanzi

- A pressure PK to solve the pressure equation.
- A saturation PK to solve the saturation equation.
- Coupled pressure PK and saturation PK (the equations are solved sequentially).
- Unit tests and convergence test for pressure equation.
Example Code for Pressure PK

// New interface for a PK
virtual void Initialize();
virtual bool AdvanceStep(double t_old, double t_new);
virtual void CommitStep(double t_old, double t_new){};
virtual void CalculateDiagnostics(){};

// Main methods of this PK
void InitializeFields();
void InitializePressure();
void InitTimeInterval(Teuchos::ParameterList& ti_list);
void CommitState(const Teuchos::Ptr<State>& S);

// Time integration interface new_mpc, implemented in Pressure_PK_TI.cc
// computes the non-linear functional f = f(t,u,udot)
virtual void Functional(double t_old, double t_new,
    Teuchos::RCP<TreeVector> u_old,
    Teuchos::RCP<TreeVector> u_new,
    Teuchos::RCP<TreeVector> f);

// applies preconditioner to u and returns the result in Pu
virtual void ApplyPreconditioner(Teuchos::RCP<const TreeVector> u,
    Teuchos::RCP<TreeVector> Pu);

// updates the preconditioner
virtual void UpdatePreconditioner(double t,
    Teuchos::RCP<const TreeVector> up, double h);
Unit test for pressure equation.

\[-\nabla \cdot (\lambda \nabla P) = f\]

Example problem

\[\lambda = 1\]
\[f = 5\pi^2 \sin (\pi x) \sin (2\pi y)\]
\[P = \sin (\pi x) \sin (2\pi y)\]
Analytic solution (left) and numeric solution (right) for test problem

\[ f(x,y) = \sin(\pi x) \cdot \sin(2\pi y) \]
Convergence rate for test problem, with mesh size $h = 8, 16, 32, 64, 128$. 

$\text{Convergence Rate}$

- $L_2$ Errors
- $h^2$
Unit test for saturation equation

- Unit test for 1D advection.

\[ u_t + f(u)_x = 0 \]

- Buckley-Leverett problem for one-dimensional 2-phase, 2-component, immiscible, incompressible flow in 1D

\[ S_t = U(S)S_x \]

\[ U(S) = \frac{Q}{\phi A} \frac{df}{dS} \]

where \( S \) is the saturation, \( Q \) is the flux, \( A \) is the surface area, \( \phi \) is the porosity, and \( f \) is the fractional flow. This is basically a nonlinear advection equation with non-convex flux \( f(S) \).
Phase I

October
- Gain confidence working with Amanzi coding standard, build tools, interfacing with other libraries, etc. ✓
- Get this new PK to interface correctly with both the multi-process coordinator (MPC) and input files. ✓
- Start with building a simple solver for the pressure equation. ✓

November
- Implement a simulator for incompressible 2-phase flow. ✓
- Fully coupled approach for incompressible 2-phase flow. ✗
- Unit tests for pressure equation. ✓
- Unit tests for saturation equation. ✗

December
- Add nonlinear complementarity constraints for phase transitions. (In progress)
- Prepare mid-year report and presentation. ✓
Phase II
- January: Develop active sets and semi-smooth Newton method.
- February: Add miscibility effect.
- March: Incorporate energy equation for thermal effect.
- April
  - Collect the unit tests and make a test suite.
  - Benchmark with existing codes or pursue realistic problems, such as desiccation if time permits.
- May: Prepare final report and presentation.

