PhD Course on
Numerical Modeling of Geological Processes
Lecture title: Mathematical models of multiphase flow

Luca Formaggia

MOX
Dipartimento di Matematica "F. Brioschi"
Politecnico di Milano

February 2013

Some definitions

- *Porous medium*: A body composed of a persistent solid part, called *solid matrix* and a *void space*, also called *pore space* that can be filled with one or more fluids.

- *Phase* A chemically homogeneous portion of a system separated from other phases by a physical boundary. In a *single-phase* system the pore space is filled by a single fluid or by several fluids completely *miscible* with each other.

- *Component* A part of a phase composed by an identifiable chemical species or assembly of species.

Main hypothesis

1. The void space of the porous medium is interconnected.
2. The dimension of the pores is large compared to the mean free path length of the fluid molecules.
3. The dimension of the pores is small enough so that the flow is controlled by adhesive forces at the fluid-solid interface and cohesive forces at the fluid-fluid interface in multiphase systems.
4. The dimensions of the pores is much smaller than those of the domain of interest (well separated scales).

These hypotheses are at the basis of the *continuum approach* and the *Darcy equation*.
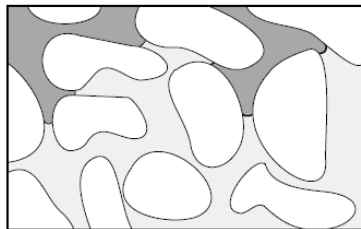
Porous media
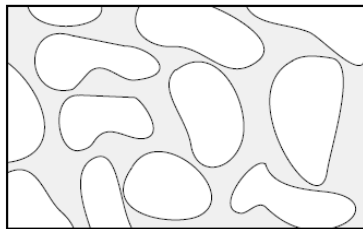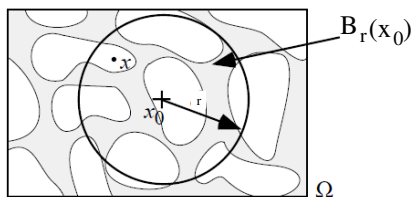

solid matrix water oil (or air)

Porosity

The definition of porosity exploits the separation of scales. Let Ω denote the domain of interest, which for simplicity we assume to cover the whole $\mathbb{R}^3$.

Let's consider at each time t the quantity

$$\chi(\mathbf{x}, t) = \begin{cases} 1 & \text{if } x \in \text{ void space} \\ 0 & \text{if } x \in \text{ solid matrix} \end{cases} \quad \mathbf{x} \in \Omega.$$

Porosity

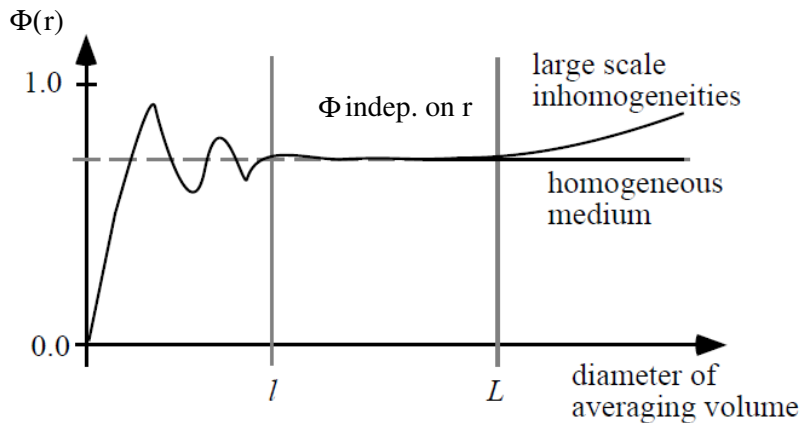At each time t we consider the function

$$\Phi(\mathbf{x}, t, r) = \int_{B_r(\mathbf{x})} \chi(\mathbf{y}, t) d\mathbf{y}$$

where $B_r(\mathbf{x})$ is the ball of radius r centered in $\mathbf{x}$. If there is a r_0 such that $|\partial_r \Phi| << 1$ for r in a neighborhood of r_0, and all $\mathbf{x}$ and t we can define a *porosity* field Φ as

$$\Phi(\mathbf{x}, t) = \Phi(\mathbf{x}, t, r_0)$$

$B_{r_0}(\mathbf{x})$ is called REV (reference elementary volume).

Example of distribution of $\Phi(r)$

Mass conservation

Let **u** be the velocity of the fluid in the porous medium and ρ the fluid density ($[kg/m^3]$). A simple balance of mass provides

$$\frac{\partial}{\partial t}(\Phi\rho) + \nabla \cdot (\rho\mathbf{u}) = \rho q \quad \text{in } \Omega, \quad t > 0.$$

where q is a possible volume source/sink ($[s^{-1}]$), to account, for instance, for a well.

Darcy's Law

Darcy's law was found experimentally in 1856 and justified later using volume averaging (Whitaker 1986) or homogenization techniques (see Hornung 1997) starting from Stokes flow at the level of the microscale.

It postulates the existence of a *absolute permeability tensor field* $\mathbf{K} = \mathbf{K}(\mathbf{x}) \in \mathbb{R}^{d \times d}$ ($[m^2]$), which is *symmetric* and *positive definite* and such that

$$\mathbf{u} = -\frac{\mathbf{K}}{\mu}(\nabla p - \rho \mathbf{g}) = -\frac{\mathbf{K}}{\mu}\rho g \nabla \Psi$$

where p ($[Pa]=[N/m^2]$) is the *fluid pressure*, $\mathbf{g} = g\mathbf{e}_z$ $[m/s^2]$ the *gravity acceleration*, μ $[Pas]$ the *dynamic viscosity*. All quantities are in fact upscaled quantities.

The quantity $\Psi = \int_{p_0}^{p} \frac{d\gamma}{\rho g} - z$ is often called *pseudo-potential*, where p_0 is a reference pressure. For incompressible fluids $\Psi = \frac{p - p_0}{\rho g} - z$ (proportional to the *piezometric head*).

Permeability
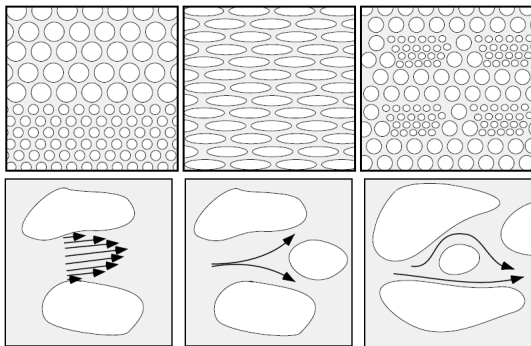
The permeability field accounts for the effect at the macroscale
level of phenomena that are intrinsically related to the microscale
level. In particular it is strongly dependent on the *tortuosity* and
connectivity of the pore space.

Darcy's equations

We then have

$$\frac{\partial}{\partial t}(\Phi\rho) - \nabla \cdot \left[\rho\frac{\mathbf{K}}{\mu}(\nabla p - \rho\mathbf{g})\right] = \rho q \quad \text{in } \Omega, \quad t > 0.$$

supplemented by initial and boundary conditions,

$$p(\mathbf{x}, 0) = p_o(\mathbf{x})$$

$$p = p_d \quad \text{on } \Gamma_d \qquad \mathbf{u} \cdot \mathbf{n} = g, \quad \text{on } \Gamma_n$$

For compressible fluids we need a constitutive relation, typically of the form $\rho = \rho(p)$ (it will usually depend on temperature).
For incompressible fluids (like when $\rho = \text{const}$), well posedness requires $|\Gamma_d| \neq 0$ (otherwise we do not have uniqueness).

Multiphase flow: saturation

Let consider a fluid with n phases. We set for any phase α

$$\chi_\alpha(\mathbf{x}, t) = \begin{cases} 1 & \mathbf{x} \in \text{phase } \alpha \\ 0 & \text{otherwise} \end{cases}$$

The *saturation* of phase α is then defined as

$$S_\alpha(\mathbf{x}, t) = \frac{\int_{B_{r_0}(\mathbf{x})} \chi_\alpha(\mathbf{y}, t) d\mathbf{y}}{\int_{B_{r_0}(\mathbf{x})} \chi(\mathbf{y}, t) d\mathbf{y}}.$$

Clearly $0 \leq S_\alpha \leq 1$, and $\sum_\alpha S_\alpha = 1$.

Conservation of mass and Darcy's law for two-phase flow

For simplicity let's consider the case of two liquid phases, a *wetting phase w* and a *non-wetting phase n* (sometimes called NAPL, Not-Aqueous Phase Liquid), with density ρ_α and moving with velocity $\mathbf{u}_\alpha$, for $\alpha \in \{w, n\}$, respectively.
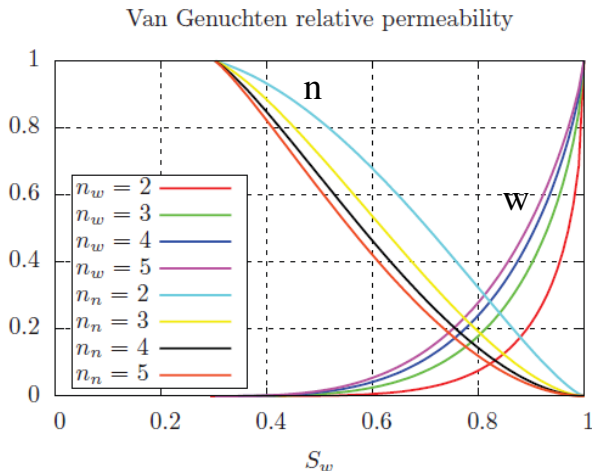
We have

$$\frac{\partial}{\partial t}(\Phi \rho_\alpha S_\alpha) + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \rho_\alpha q_\alpha$$

with $\mathbf{u}_\alpha = -\lambda_\alpha \mathbf{K}(\nabla p_\alpha - \rho_\alpha \mathbf{g})$

$\lambda_\alpha = \frac{k_\alpha}{\mu_\alpha}$ is the *mobility*, and k_α the *relative permeability* of phase α, with $0 \le k_\alpha \le 1$.

Relative permeability curves

Van Genuchten relative permeability

At low saturation the relative permability is low since the fluid has to "find its way" through the other fluid. In fact the curve may be different in drainage/filling and may exhibit *hysteresis effects*.

Capillarity effects

A main issue in multiphase flow are the capillary forces arising at the sharp interface between phases.
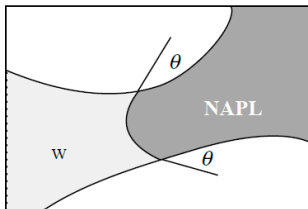
Capillary forces depend on the characteristics of the two fluids, the saturation, the distribution of pore sizes.

It is normally accepted to postulate the existence of a *non-negative field* $p_c = p_c(S_w)$ called *capillary pressure*, such that $p_n - p_w = p_c$.

Capillary pressure curves

Van Genuchten capillary pressure
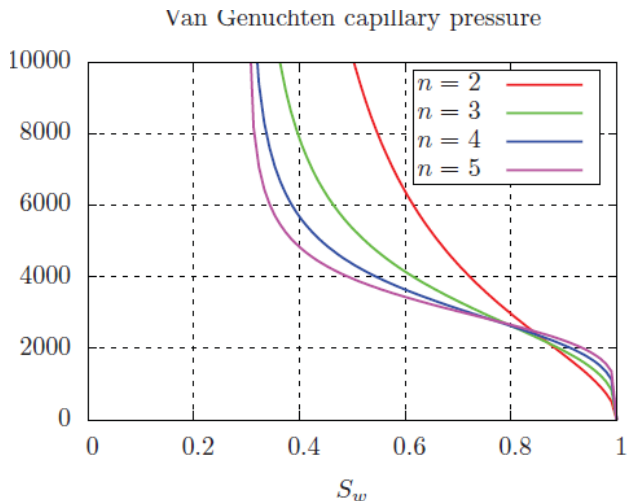
$p_s(S_w) = \frac{1}{\alpha} \left(\overline{S}_w^{\frac{n}{1-n}} - 1 \right)^{\frac{1}{n}}$ with $\overline{S}_w = \frac{S_w - S_{w,r}}{1 - S_{w,r} - S_{n,r}}$, $S_{\alpha,r}$ being the *residual saturations*

Equations in saturation-pressure form

$$\begin{cases} \frac{\partial}{\partial t}(\Phi \rho_\alpha S_\alpha) + \nabla \cdot (\rho_\alpha \mathbf{u}_\alpha) = \rho_\alpha q_\alpha & \alpha = \{w, n\} \\ \mathbf{u}_\alpha = -\lambda_\alpha(S_w)\mathbf{K}(\nabla p_\alpha - \rho_\alpha \mathbf{g}) \\ S_w + S_n = 1 \\ p_n - p_w = p_c(S_w) \end{cases}$$

Equations are rarely solved in this form because of the complexity of imposing the algebraic constraints. We will derive an alternative formulation that also enlightens the mathematical characteristic of this system of equations.

Total pressure formulation

Even if it is possible to derive the formulation in the more general case, for the sake of simplicity we limit ourselves to two-phase incompressible flows and we assume that the porosity does not depend on time (compaction processes are negligible).
We can simplify the previous set of equations into

$$
\begin{cases}
\Phi \frac{\partial}{\partial t} S_\alpha + \nabla \cdot \mathbf{u}_\alpha = q_\alpha,\ \alpha = \{w, n\}, & S_w + S_n = 1, \\
\mathbf{u}_\alpha = -\lambda_\alpha(S_w)\mathbf{K}(\nabla p_\alpha - \rho_\alpha \mathbf{g}), & p_n - p_w = p_c(S_w).
\end{cases}
\tag{1}
$$

We also make the assumption that mobilities and capillary pressure depend on S_w only.

Global pressure formulation

- Total mobility $\lambda = \lambda_w + \lambda_n$;
- Modified gravity $\mathbf{G} = \mathbf{g} \frac{\rho_w \lambda_w + \rho_n \lambda_n}{\lambda}$;
- Capillary pressure derivative $p_c'(S_w) = \frac{d}{dS_w} p_c(S_w)$.
- Fractional Flow. $f_\alpha = \lambda_\alpha / \lambda$ (is a function of S_w).
- Total velocity $\mathbf{u} = \mathbf{u}_n + \mathbf{u}_w$;
- Global pressure $p(\mathbf{x}, t; S_w) = p_n(\mathbf{x}, t) - \pi_w(S_w)$, with

$$\pi_w(S) = \int_{S_0}^{S} f_w(\gamma) p_c'(\gamma) d\gamma.$$

Note that if $p_c' = 0$ then $p = p_n$.

Global pressure formulation

With a few manipulation one finds that system (1) is equivalent to

$$
\begin{cases}
\nabla \cdot \mathbf{u} = q_n + q_w \\
\mathbf{u} = -\lambda \mathbf{K}(\nabla p - \mathbf{G}) \\
\Phi \frac{\partial}{\partial t} S_w + \nabla \cdot \mathbf{u}_w = q_w \\
\mathbf{u}_w = f_w \mathbf{u} + \lambda_n(S_w) f_w(S_w) \mathbf{K} \left[p_c'(S_w) \nabla S_w + (\rho_w - \rho_n) \mathbf{g} \right]
\end{cases}
\tag{2}
$$

Note that the last two equations imply that S_w satisfies an equation of the type

$$
\Phi \frac{\partial}{\partial t} S_w + \nabla \cdot F(S_w) + \nabla \cdot \left[\lambda_n(S_w) f_w(S_w) p_c'(S_w) \nabla S_w \right] + B(S_w) = 0
$$

which is a possibly degenerate non-linear parabolic equation. If the diffusive term vanishes we have an hyperbolic equation for the saturation.

Typical boundary conditions

$$
\begin{cases}
S = S^g & \text{on } \Gamma_d^S \\
\frac{\partial}{\partial n} S = h & \text{on } \Gamma_n^S \\
p = g & \text{on } \Gamma_d^p \\
\rho_w \mathbf{u}_w \cdot \mathbf{n} = F & \text{on } \Gamma_n^p
\end{cases}
\qquad \text{for } t > 0
$$

In the degenerate hyperbolic case Dirichlet conditions for S_w may be applied only on inflow boundary, we will deal with this issue later on.

We need an initial condition for S_w at time $t = 0$. For the compressible case we need also an initial condition for pressure.

Solution schemes

There are basically two ways of addressing the problem. Either with a monolithic scheme that treats the non-linear system as a whole, or by using a operator splitting strategy that separates the equations for the pressure/velocity from that of the saturation.

A popular splitting strategy is the IMPES scheme (implicit pressure/explicit saturation): At each time step

- ▶ Solve the fist two equation by keeping the saturation fixed at the value calculated at the previous time step using an implicit scheme;

- ▶ Advance the saturation using an explicit or a semi-implicit scheme, possibly subiterating for stability reasons, using the computed value of the Darcy velocity.

Main computational issues

- **Transport dominated** (possibly degenerate) parabolic problem for the saturation. Centered methods do not work well in this case. We need upwind stabilization.

- **Coupled problem**. The multiphase flow equations are a non-linear coupled system of equations. The pressure has always to be treated implicitely (necessary in the incompressible case, in the compressible case an explicit treatment will impose too restrictive time-step constraints).

- **Accurate flow velocity**. The coupling between the pressure-velocity equation and the saturation equation is through the velocity. While pressure may vary considerably, the total velocity is normally relatively smooth. If we use the pressure equation and reconstruct the velocity through the Darcy's law results in a less accurate velocity, particularly if permeability or viscosity vary a lot in the domain.

Main computational issues

- In situations like viscous fingering the boundary between phases should be reconstructed accurately,

- Large size problems. For realistic situations we may have millions of degrees of freedom. Iterative methods are in this case mandatory, which calls for proper preconditioners. An ideal preconditioner should make the number of iteration to convergence constant with respect to the grid size h, the jump in the coefficients μ_{max}/μ_{min} etc., and, in parallel computations, the ratio between the number of processors and the mesh size (weak scalability). This is partially still a subject of research.