Phase exchange for flow in porous media and complementary problems

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Dedicated to Alain Bourgeat

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Motivation : Couplex-Gas, an Andra-Momas benchmark

- In a deep underground nuclear waste disposal
- Production of hydrogen from corrosion of waste packets
- Migration of this hydrogen ?

Formulations with complementary equations can be found in

G. Chavent and J. Jaffré, Mathematical models and finite elements for reservoir simulation, (North Holland, 1986)

A. Bourgeat, M. Jurak and F. Smaï, Two phase partially miscible flow and transport modeling in porous media ; application to gas migration in a nuclear waste repository

A recent work with a new formulation:

A. Abadpour and M. Panfilov, Method of negative saturations for multiple compositional flow with oversaturated zones.

Formulation I: Phase equations

2 fluid phases: liquid ($i = \ell$) and gas ($i = g$)

Darcy's law: $\mathbf{q}_i = -K(x)k_i(s_i)(\nabla p_i - \rho_i g \nabla z), \quad i = \ell, g$

K the absolute permeability
$\mathbf{q}_i$ Darcy's velocities, s_i saturations, p_i fluid pressures, k_i mobilities

Phases occupy the whole pore space: $s_\ell + s_g = 1$.

Capillary pressure law: $p_c(s_\ell) = p_g - p_\ell \geq 0$, p_c decreasing, $p_c(1) = 0$.

Since liquid phase does not disappear, main unknowns will be s_ℓ and p_ℓ.

Fluid components

2 components: water ($j = w$) and hydrogen ($j = h$).

Mass density of phase i: $\rho_i = \rho_w^i + \rho_h^i, \quad i = \ell, g$.

Mass fractions: $\chi_h^i = \dfrac{\rho_h^i}{\rho_i}, \quad \chi_w^i = \dfrac{\rho_w^i}{\rho_i}, \quad i = \ell, g, \quad (\chi_w^i + \chi_h^i = 1)$.

Assume
- liquid phase contains both components,
- gas phase contains only hydrogen.

Then $\rho_w^g = 0, \quad \rho_g = \rho_h^g, \quad \chi_h^g = \dfrac{\rho_h^g}{\rho_g} = 1, \quad \chi_w^g = 0$.

Assume
- $\rho_g = C_g p_g$ and ρ_w^ℓ constant.

χ_h^ℓ is the third main unknown.

Conservation of components

Diffusion of hydrogen in the liquid phase:

$$j_h^\ell = -\phi s_\ell \rho_\ell D_h^\ell \nabla \chi_h^\ell.$$

ϕ porosity, D_h^ℓ molecular diffusion coefficient.

Mass conservation for each component:

Water: $$\phi \frac{\partial}{\partial t}(s_\ell \rho_\ell \chi_w^\ell) + \mathrm{div}(\rho_\ell \chi_w^\ell \mathbf{q}_\ell) = Q_w$$

Hydrogen: $$\phi \frac{\partial}{\partial t}(s_\ell \rho_\ell \chi_h^\ell + s_g \rho_g) + \mathrm{div}(\rho_\ell \chi_h^\ell \mathbf{q}_\ell + \rho_g \mathbf{q}_g + j_h^\ell) = Q_h.$$

Phase equilibrium: Henry's law

In the presence of gas phase Henry's law reads $Hp_g = \rho_h^\ell$.

To integrate Henry's law in a formulation which includes the case with no gas phase, introduce the liquid pressure $p_\ell = p_g - p_c(s_\ell)$, and

- Either gas phase exists: $1 - s_\ell > 0$ and $H(p_\ell + p_c(s_\ell)) - \rho_h^\ell = 0$
- Or gas phase does not exist: $s_\ell = 1, p_c(s_\ell) = 0$ and $Hp_\ell - \rho_h^\ell \geq 0$

In other words, last inequality means

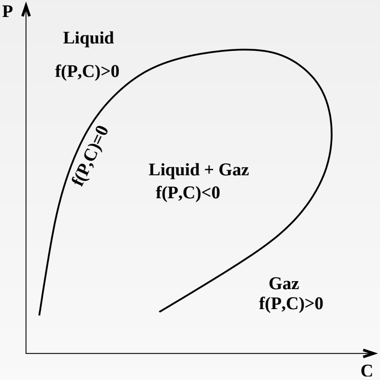
- for a given pressure p_ℓ mass fraction is too small for the hydrogen component to be partly gaseous,
- for a given mass fraction ρ_h^ℓ the pressure p_ℓ is too large for the hydrogen component to be partly gaseous.

Thus we close the system with the complementary constraints

$$(1-s_\ell)\Big(H(p_\ell+p_c(s_\ell))-\rho_h^\ell\Big) = 0, \quad 1-s_\ell \geq 0, \quad H(p_\ell+p_c(s_\ell))-\rho_h^\ell \geq 0.$$

Phase diagram

A phase diagram tells also how a component separates into the liquid and gas phases:

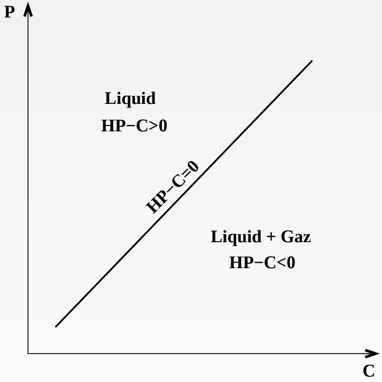


	liquid	liquid + gas	gas
	$s_\ell = 1$	$0 < s_\ell < 1$	$s_\ell = 0$
P	p_ℓ	$p_g = p_\ell - p_c(s_\ell)$	p_g
C	ρ_h^ℓ	$\rho_h^\ell + \rho_g$	ρ_g

We now concentrate on the separation one liquid phase – twophase zones.

Henry's law versus phase diagram

- In the twophase zone, with Henry's law
$$HP - C = Hp_g - (\rho_h^\ell + \rho_g) = -\rho_g < 0.$$
- When moving to the separation between liquid and twophase zones
$$HP - C = -\rho_g \to 0.$$
- In the liquide zone $HP - C = Hp_\ell - \rho_h^\ell > 0.$



	liquid	liquid + gas
	$s_\ell = 1$	$0 < s_\ell < 1$
P	p_ℓ	$p_g = p_\ell - p_c(s_\ell)$
C	ρ_h^ℓ	$\rho_h^\ell + \rho_g$

Thus, with Henry's law, the curve separating the liquid and twophase zones is the straight line $HP - C = 0$.

A nonlinear problem with complementary equations

$$\phi\frac{\partial}{\partial t}\big(s_\ell\rho_\ell(1-\chi_h^\ell)\big)+\operatorname{div}\big(\rho_\ell(1-\chi_h^\ell)\mathbf{q}_\ell\big)=Q_w$$

$$\phi\frac{\partial}{\partial t}\big(s_\ell\rho_\ell\chi_h^\ell+(1-s_\ell)C_g(p_\ell+p_c(s_\ell))\big)+$$
$$\operatorname{div}\big(\rho_\ell\chi_h^\ell\mathbf{q}_\ell+C_g(p_\ell+p_c(s_\ell))\mathbf{q}_g+j_h^\ell\big)=Q_h$$

$$\mathbf{q}_\ell=-K(x)k_\ell(s_\ell)(\nabla p_\ell-\rho_\ell g\nabla z)$$

$$\mathbf{q}_g=-K(x)k_g(1-s_\ell)(\nabla(p_\ell+p_c(s_\ell))-C_g(p_\ell+p_c(s_\ell))g\nabla z)$$

$$j_h^\ell=-\phi s_\ell\rho_\ell D_h^\ell\nabla\chi_h^\ell$$

$$(1-s_\ell)\big(H(p_\ell+p_c(s_\ell))-\rho_\ell\chi_h^\ell\big)=0,\quad 1-s_\ell\geq 0,$$
$$H(p_\ell+p_c(s_\ell))-\rho_\ell\chi_h^\ell\geq 0.$$

The discretized problem

Discretized with cell-centered finite volumes : N, the number of cells.

$x \in \mathbb{R}^{3N}$, vector of unknowns for $s_\ell, p_\ell, \chi_h^\ell$

$\mathcal{H} : \mathbb{R}^{3N} \to \mathbb{R}^{2N}$ for discretized conservation equations

$\mathcal{F} : \mathbb{R}^{3N} \to \mathbb{R}^{N}$ for discretized $1 - s_\ell$

$\mathcal{G} : \mathbb{R}^{3N} \to \mathbb{R}^{N}$ for discretized $H(p_\ell + p_c(s_\ell)) - \rho_\ell \chi_h^\ell$

Problem in compact form

$$\mathcal{H}(x) = 0,$$
$$\mathcal{F}(x)^\top \mathcal{G}(x) = 0, \quad \mathcal{F}(x) \geq 0, \quad \mathcal{G}(x) \geq 0.$$

Task

$$\mathcal{H}(x) = 0,$$
$$\mathcal{F}(x)^\top \mathcal{G}(x) = 0, \quad \mathcal{F}(x) \geq 0, \quad \mathcal{G}(x) \geq 0.$$

Construction of general purpose fast and robust solvers for nonlinear problems with complementary constraints

Additional difficulties:

- Unknowns s_ℓ and χ_h^ℓ are bounded
- Vertical tangent of p_c at $s = 1$ in the Van Genuchten model

Other examples for flow in porous media

- Black-oil model
- Dissolution-precipitation