A tri-phase phase-field model for precipitation and dissolution in partially saturated porous media

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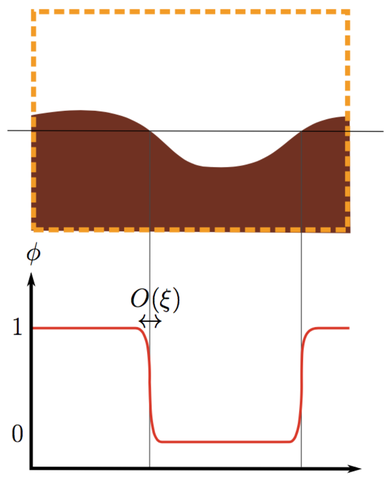
Introduction

- Dissolution/precipitation, unsaturated porous media: pore geometry changes.
- Changes not known a-priori, **evolving interfaces at the pore scale**.
- Modelling: characteristic functions or level sets locating the interfaces.
- Alternative: **phase fields**.
- Interfaces $\to$ ϵ-thick diffuse layers.
- Research questions:
  - Sharp interface model when $\epsilon \searrow 0$?
  - Upscaling: **Darcy scale** model?
  - Efficient simulation method?

Phase fields



Phase fields: approximate interfaces by thin diffuse layers.
Evolution: Allen-Cahn, or Cahn-Hilliard equation.

Conclusions

- ∗ Pore scale model: water, air in the void space, precipitate at the pore walls.
- ∗ Phase field modelling: fixed domains, evolving interfaces replaced by thin diffusion layers.
- ∗ Homogenization: Darcy scale model.
- ∗ Efficient multi-scale adaptive scheme.
- ∘ Future work: include flow, contact angles, variable surface tension effects.

References

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Dissolution/precipitation in unsaturated porous media

The phase field model

Unknowns (defined for $t > 0$, $x \in \mathcal{P}_\delta$):
$u \in [0, \rho]$: solute concentration
$\mathbf{\Phi} = (\phi_1, \phi_2, \phi_3) \in [0,1]^3$: phase indicators

In $\mathcal{P}_\delta$:

$$\partial_t(\phi_1 u) - \nabla \cdot (\phi_1 D \nabla u) = \rho \frac{\phi_3}{1-\phi_1} \partial_t \phi_1,$$

$$\alpha \epsilon^2 \partial_t \phi_i - \frac{3}{4}\epsilon^2 \Delta \phi_i = -G_i(\mathbf{\Phi}, u),$$

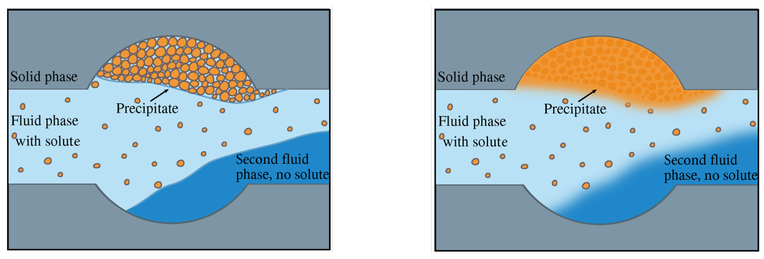
for $i = 1, 2, 3$, and no flow at $\partial \mathcal{P}_\delta$. Here:

$$G_i(\mathbf{\Phi}, u) = f_i(\mathbf{\Phi}, u) + \sum_{j \neq i} (\partial_{\phi_i} - \partial_{\phi_j}) W(\mathbf{\Phi}),$$

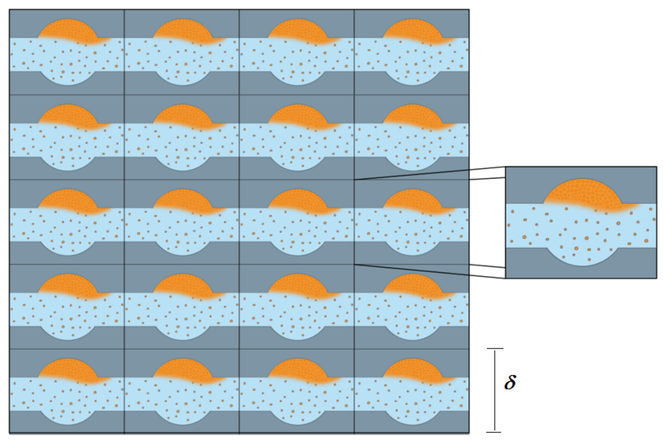
$$W(\mathbf{\Phi}) = 2 \sum_{i=1,2,3} \phi_i^2 (1-\phi_i)^2, \; f_2(\mathbf{\Phi}, u) = 0,$$

$$f_1(\mathbf{\Phi}, u) = -f_3(\mathbf{\Phi}, u) = 4\alpha\epsilon\phi_1\phi_3 f(u),$$

and f models the precipitation/dissolution.



Interfaces vs. diffuse layers, pore scale.



Unsaturated, periodic porous medium.

Results

Pore scale model:

- Existence and uniqueness of solutions for the (decoupled) model, $\phi_i \in [0,1]$ a.e.
- Decreasing free energy $U(\mathbf{\Phi}) = 3\int_{\mathcal{P}_\delta} W(\mathbf{\Phi}) + \frac{3}{8}\epsilon^2 \sum \|\nabla \phi_i\|^2$.
- Limit $\epsilon \searrow 0$ leads to the sharp interface model (with curvature effects).

Upscaling for a periodic domain ($\delta = O(\epsilon)$, $\alpha = O(\epsilon^{-2})$, $f_i \to \delta f_i$):

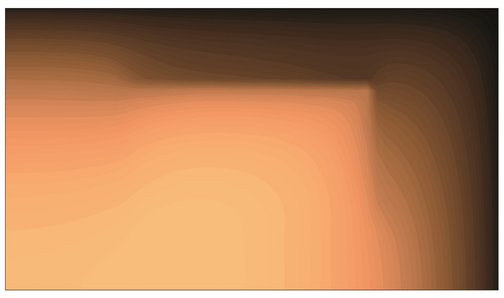
- **Darcy scale model** (regularised), uses doubling of variables $y = \frac{1}{\delta}x$:

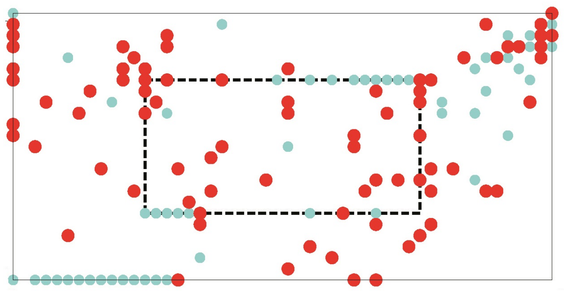
$$\partial_t\left(\overline{\phi_1}^{\mathcal{P}} u\right) - D\nabla_x \cdot \left(K(\phi_1)\nabla_x u\right) = \rho \overline{g(\mathbf{\Phi})\partial_t \phi_1}^{\mathcal{P}},$$

where $\left(K(\phi_1)\right)_{ij} = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \phi_1(\delta_{ij} + \partial_{y_i} w_j)dy$, $\overline{\phi_1}^{\mathcal{P}} = \frac{1}{|\mathcal{P}|}\int_{\mathcal{P}} \phi_1(t,x,y)dy$, and $g(\mathbf{\Phi}) = \frac{\phi_3}{1-\phi_1}$. Here ϕ_1 and w_j solve the *periodic cell problems* in $\mathcal{P}$ ($j = 1, 2$):

$$\alpha_0 \epsilon_0^2 \partial_t \phi_i - \frac{3}{4}\epsilon_0 \Delta_y \phi_i = -G_i(\mathbf{\Phi}, u),$$
$$-D\nabla_y \cdot (\phi_1 \nabla_y w_j) = D\nabla_y \cdot (\phi_1 \mathbf{e}_j).$$

- **Adaptive** multi scale algorithm, effective parameters computed only for *active* macro-scale nodes. These are updated every time step depending on a *tolerance*.





$c_{\mathrm{tol_r}}$	$\|\Delta u\|_{J\times\Omega,\infty}$	$\|\Delta u\|_{J\times\Omega,2}$	$\overline{\lvert N_A \rvert}$
1	$5.64e-03$	$2.70e-03$	4.00
$10^{-1/2}$	$2.57e-02$	$2.68e-03$	6.33
10^{-1}	$1.60e-03$	$2.30e-04$	14.45
$10^{-3/2}$	$6.08e-04$	$2.26e-04$	28.84
10^{-2}	$8.59e-05$	$3.44e-05$	38.57
0	$0.00e{+}0$	$0.00e{+}0$	81.00

Test case: (L) Low initial solute concentration, much salt present in the middle. (M) Active nodes (red) and nodes set to inactive (blue). (R) Error decay and $\overline{N_A}$ - averaged number of active nodes (out of 1250), depending on the tolerance.

Acknowledgements

Research supported by the Research Foundation Flanders (FWO), Belgium, through the *Odysseus* programme, Project G0G1316N **"DynScale"**.

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