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 $\rightarrow$ $\epsilon$-thick diffuse layers.
- Research questions:
  - Sharp interface model when $\epsilon \searrow 0$?
  - Upscaling: Darcy scale model?
  - Efficient simulation method?

**Phase fields**


**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**

**Dissolution/precipitation in unsaturated porous media**

The phase field model

$\Phi = (\phi_1, \phi_2, \phi_3) \in [0, 1]^3$: phase indicators

In $\mathcal{P}$:

$$
\partial_t (\phi_1 u) - \nabla \cdot (\rho \phi_1 \mathbf{1} - \mathbf{1} \phi_1) = 0,
$$

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

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

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

$$
W(\Phi) = 2 \sum_{i=1,2,3} \phi_i^4 (1 - \phi_i)^2, f_2(\Phi, u) = 0,
$$

$$
f_1(\Phi, u) = -f_3(\Phi, u) = 4 \alpha \epsilon \phi_i f(u),
$$

and $f$ models the precipitation/dissolution.

**Results**

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

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

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

$$
\partial_t (\bar{\phi}_i^p) - D \nabla \cdot (K(\bar{\phi}_1) \nabla \bar{\phi}_i) = pg(\bar{\Phi}) \partial_{\phi_i} \bar{\phi}_i^p,
$$

where $(K(\bar{\phi}))^p_{ij} = \frac{1}{\epsilon} \int_{\mathcal{P}} \phi_i (\delta_{ij} + \partial_{\phi_j} w_j) dy$, $\bar{\phi}_i^p = \frac{1}{\epsilon H} \int_{\mathcal{P}} \phi_i (t, x, y) dy$, and $g(\bar{\Phi}) = \frac{\phi_i}{\epsilon H}$. Here $\phi_i$ and $w_j$ solve the periodic cell problems in $\mathcal{P}$ ($j = 1, 2$):

$$
\alpha \epsilon \phi_i^2 \partial_{\phi_i} \phi_i - \frac{3}{4} \epsilon^2 \nabla \phi_i = -G_i(\bar{\Phi}, u),
$$

$$
- D \nabla \cdot (\phi_i \nabla w_j) = D \nabla \cdot (\phi_i \phi_j).
$$

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

**Acknowledgements**

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 $N_A$ avgeraged number of active nodes (out of 1250), depending on the tolerance.

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