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Finding a balance between accuracy and effort for modeling biomineralization

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Motivation

With increasing intensity of subsurface use, ensuring separation between different layers with competitive uses becomes more and more important. To ensure separation, sealing technologies such as microbially induced calcite precipitation (MICP) are important. This and other applications of MICP are discussed in Phillips et al. [3].

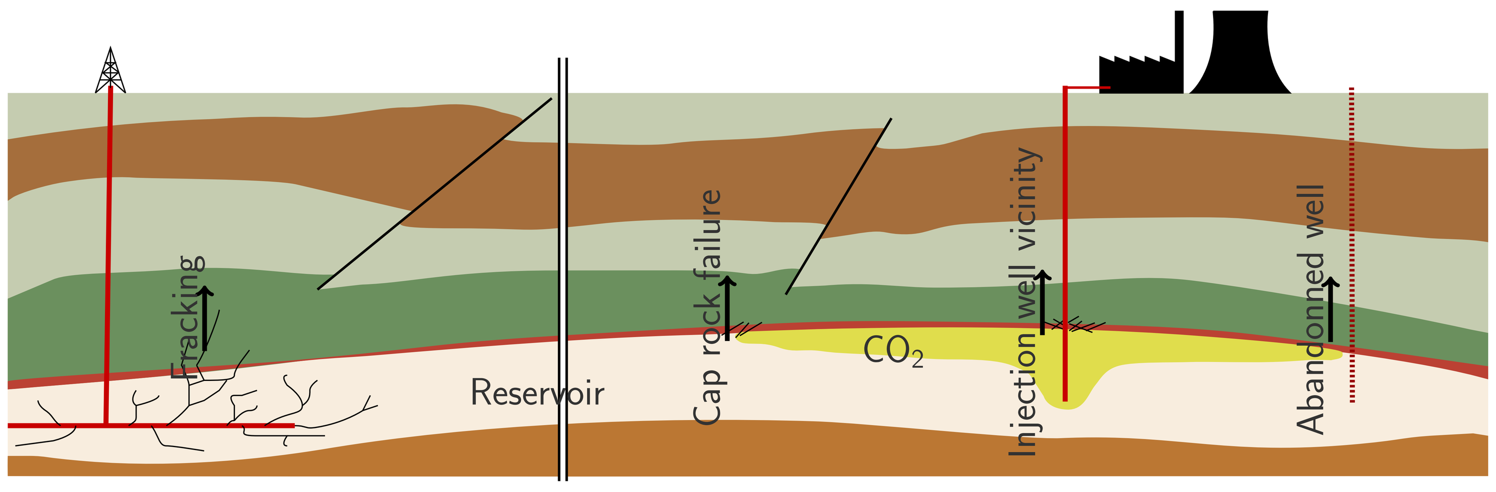

Figure 1 : *Potential application sites of MICP as a sealing technology in the subsurface.*

Field-scale MICP simulations are prohibitively computationally expensive.
⇒ **Need for a reduction of the computational effort, while preserving as much accuracy as possible.**

Model Concept

The REV-scale MICP model includes reactive two-phase multi-component transport including two solid phases.

$$\text{solid phases: } \frac{\partial}{\partial t}(\phi_\lambda \rho_\lambda) = q^\lambda_{\text{reactions}}$$

$$\text{solutes: } \sum_\alpha \left[\frac{\partial}{\partial t}(\phi \rho_\alpha x^\kappa_\alpha S_\alpha) + \nabla\cdot(\rho_\alpha x^\kappa_\alpha \mathbf{v}_\alpha) - \nabla\cdot(\rho_\alpha \mathbf{D}_{\text{pm},\alpha} \nabla x^\kappa_\alpha)\right] = q^\kappa_{\text{reactions}}$$

Relevant processes

- two-phase multi-component flow
- processes determining the distribution of biomass:
  - growth: $r_{\text{growth}} = \mu\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}} \frac{C_w^{O_2}}{C_w^{O_2}+K_{O_2}} \frac{C_w^{\text{substrate}}}{C_w^{\text{substrate}}+K_{\text{substrate}}}$,
  - decay: $r_{\text{decay}} = k_{\text{decay}}\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}}$,
  - attachment: $r_{\text{attachment}} = (c_{a,1}\, \phi_{\text{biofilm}} + c_{a,2})\, S_w\, \phi\, C_w^{\text{bacteria}}$,
  - detachment: $r_{\text{detachment}} = c_{d,1}\, (S_w\, \phi\, |\nabla p_w|)^{0.58} + c_{d,2}\, \mu$,
- (bio-) chemical reactions:
  - microbially catalyzed ureolysis: $CO(NH_2)_2 + 2\,H_2O \xrightarrow{\text{urease}} 2\,NH_3 + H_2CO_3$,
    $r_{\text{urea}} = k_{\text{urease}}\, k_{\text{ub}}\, \rho_{\text{biofilm}}\, \phi_{\text{biofilm}} \frac{m^{\text{urea}}}{m^{\text{urea}}+K_{\text{urea}}}$.
  - influence of NH_3 on the pH: $NH_3 + H^+ \leftrightarrow NH_4^+ \Rightarrow$ increase in pH,
  - precipitation (and dissolution) of calcite: $Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_3 \downarrow$,
    $r_{\text{precipitation}} = k_{\text{precipitation}}\, A_{\text{sw}}\, (\Omega - 1)^{n_{\text{precipitation}}}$,
    which is depended on the calcite saturation state $\Omega = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{\text{sp}}}$ and the water-solid surface area A_{sw}.
- clogging: $\phi = \phi_0 - \phi_{\text{calcite}} - \phi_{\text{biofilm}} \Rightarrow K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}}\right)^3$

Setup

The setup is the bicycle rim experiment described in Hommel et al. [2].

- compare heterogeneous and homogeneous case
- relate the error due to assuming homogeneity to the model simplifications

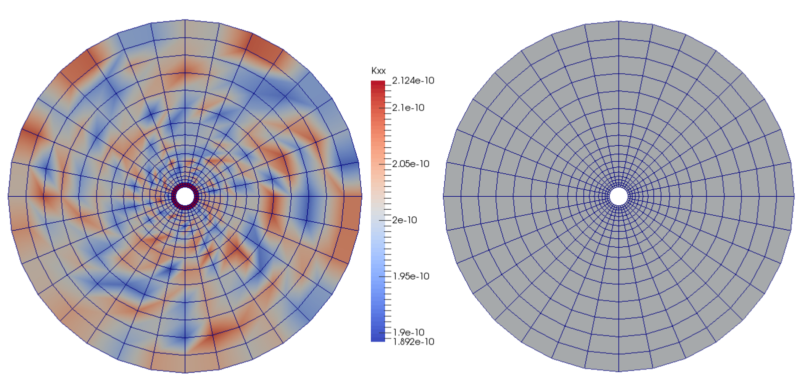

Figure 2 : *Heterogeneous and homogeneous permeability used to calculate a base error to compare with the error of the model simplifications.*

Model simplification

The **full complexity model (FC)** and two simplifications are investigated:

Initial biofilm (IB):
Instead of an inoculation period, the model is started at a later time with a pre-established biofilm. The component suspended biomass is neglected [1], resulting in a reduced number of unknowns.

Simple chemistry (SC):
Activities and saturation index are neglected, the precipitation rate is assumed to be equal to the ureolysis rate as in e.g. van Wijngaarden et al. [4], $r_{\text{prec}} = r_{\text{urea}}$. This model has the full set of unknowns, but the geochemistry is neglected.

Results

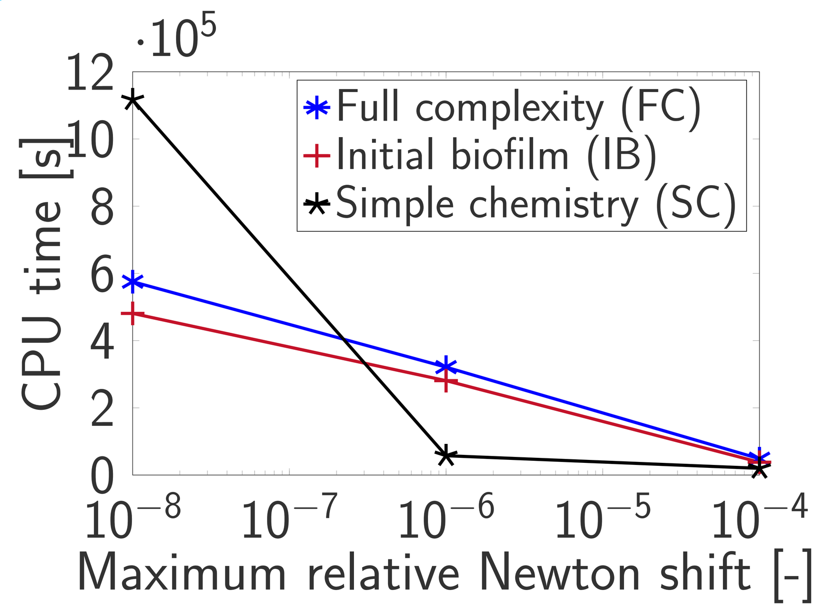

Figure 3 : *CPU times for simplified models for various Newton tolerances.*

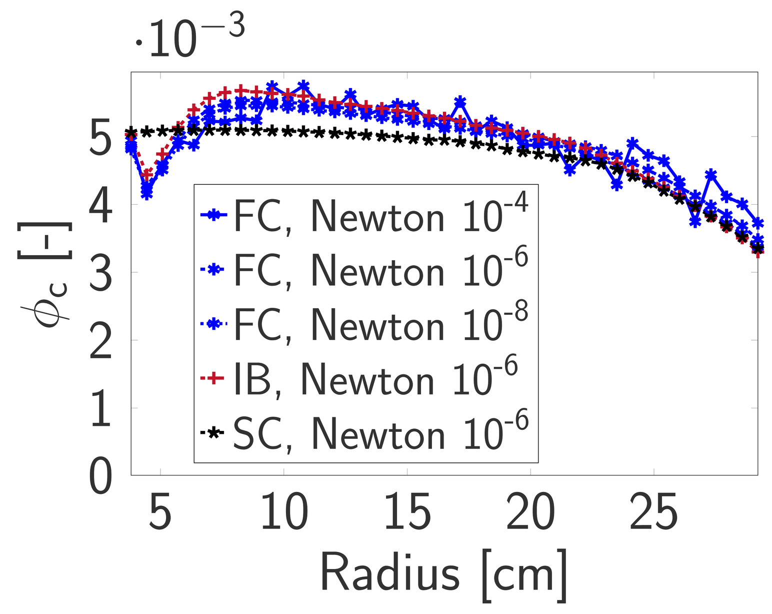

Figure 4 : *Predictions of precipitated calcite after model simplifications.*

Table 1 : *Comparison of the simplified models. Reference error homogeneous to heterogeneous permeability: 0.0033.*

Model	CPU time	Error	Newton it.	Lin. it. / N. it
FC, N 10^{-6}	32110 s	0.0025	4971	15.15
FC, N 10^{-4}	4861 s	0.0065	776	6.57
SC, N 10^{-6}	5758 s	0.0070	1094	14.90
SC, N 10^{-4}	2001 s	0.0104	396	13.14
IB, N 10^{-6}	28089 s	0.0040	5053	14.9

- **Relaxing the Newton convergence criterion is a simple but effective measure to reduce CPU time.**
- For the given setup, the CPU time of the **simple chemistry model (at N 10^{-6}) is comparable** to relaxing the Newton convergence criterion.
- The simple chemistry model **could be simplified further, removing additionally the components suspended biomass** (see IB model) and **Na^+, Cl^-**, and **NH_4^+**, as the geochemistry is neglected in this setup.

Literature

[1] Hommel, J., Lauchnor, E., Gerlach, R., Cunningham, A. B., Ebigbo, A., Helmig, R., and Class, H. (2016). Investigating the influence of the initial biomass distribution and injection strategies on biofilm-mediated calcite precipitation in porous media. *Transport in Porous Media*, 114(2):557–579.

[2] Hommel, J., Lauchnor, E. G., Phillips, A. J., Gerlach, R., Cunningham, A. B., Helmig, R., Ebigbo, A., and Class, H. (2015). A revised model for microbially induced calcite precipitation: Improvements and new insights based on recent experiments. *Water Resources Research*, 51(5):3695–3715.

[3] Phillips, A. J., Gerlach, R., Lauchnor, E. G., Mitchell, A. C., Cunningham, A. B., and Spangler, L. H. (2013). Engineered applications of ureolytic biomineralization: a review. *Biofouling*, 29(6):715–733.

[4] van Wijngaarden, W. K., Vermolen, F. J., Meurs, G. A. M., and Vuik, C. (2013). A mathematical model for Biogrout. *Computational Geosciences*, 17(3):463–478.