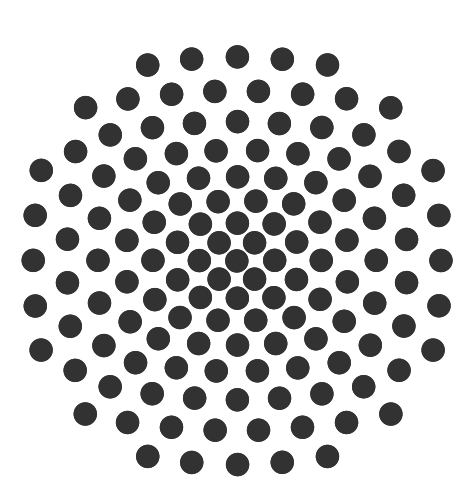
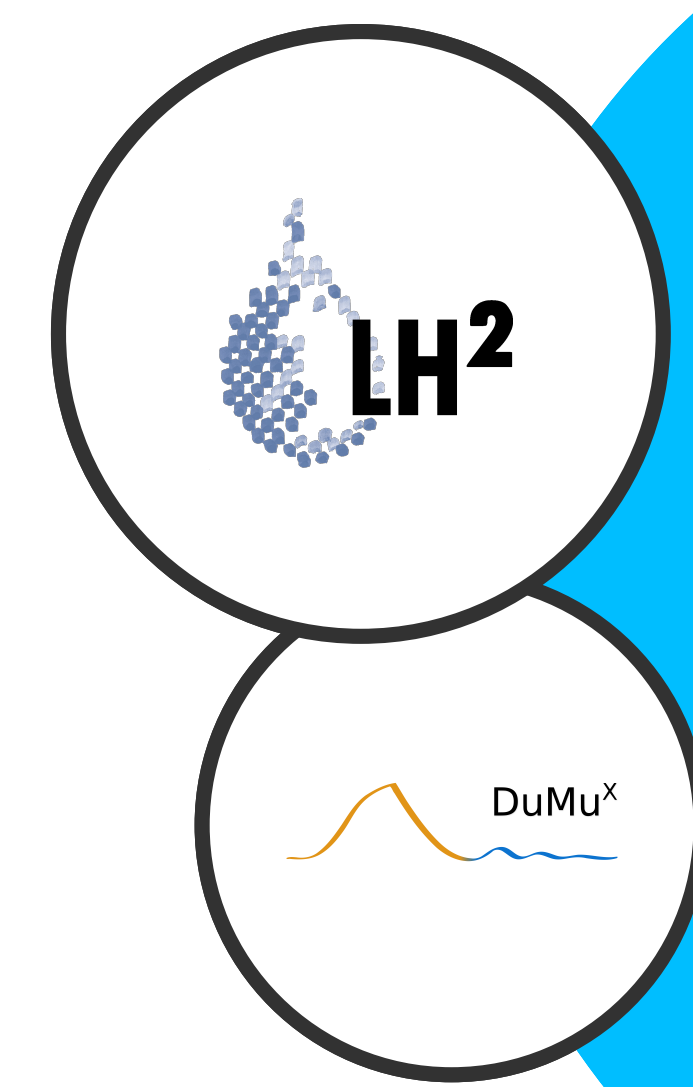




Finding a balance between accuracy and effort for modeling biomineralization

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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].

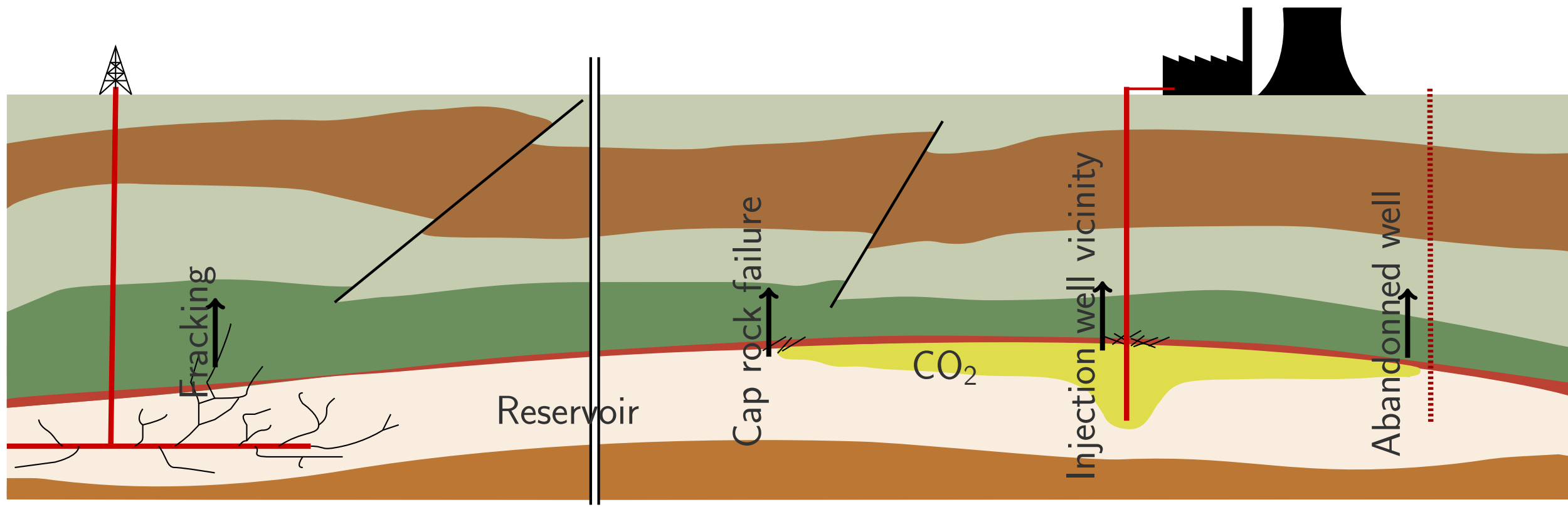


Figure 1 : Potential application sites of MICP as a sealing technology in the subsurface.

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.**

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

$$\text{solute: } \sum_\alpha \left[\frac{\partial}{\partial t} (\phi_\alpha x_\alpha^\kappa S_\alpha) + \nabla \cdot (\rho_\alpha x_\alpha^\kappa \mathbf{v}_\alpha) - \nabla \cdot (\rho_\alpha \mathbf{D}_{\text{pm},\alpha} \nabla x_\alpha^\kappa) \right] = q_{\text{reactions}}^\kappa$$

Relevant processes

- two-phase multi-component flow
- processes determining the **distribution of biomass**:
 - growth**: $r_{\text{growth}} = \mu \rho_{\text{biofilm}} \phi_{\text{biofilm}} \frac{C_{\text{O}_2}}{C_{\text{O}_2} + K_{\text{O}_2}} \frac{C_{\text{substrate}}}{C_{\text{substrate}} + K_{\text{substrate}}}$,
 - decay**: $r_{\text{decay}} = k_{\text{decay}} \rho_{\text{biofilm}} \phi_{\text{biofilm}}$,
 - attachment**: $r_{\text{attachment}} = (c_{a,1} \phi_{\text{biofilm}} + c_{a,2}) S_w \phi C_{\text{bacteria}}$,
 - 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**: $\text{CO}(\text{NH}_2)_2 + 2\text{H}_2\text{O} \xrightarrow{\text{urease}} 2\text{NH}_3 + \text{H}_2\text{CO}_3$,
 - $r_{\text{urea}} = k_{\text{urease}} k_{\text{ub}} \rho_{\text{biofilm}} \phi_{\text{biofilm}} \frac{m_{\text{urea}}}{m_{\text{urea}} + K_{\text{urea}}}$,
 - influence of NH_3 on the pH: $\text{NH}_3 + \text{H}^+ \leftrightarrow \text{NH}_4^+ \Rightarrow \text{increase in pH}$,
 - precipitation** (and dissolution) of **calcite**: $\text{Ca}^{2+} + \text{CO}_3^{2-} \leftrightarrow \text{CaCO}_3 \downarrow$,
 - $r_{\text{precipitation}} = k_{\text{precipitation}} A_{\text{sw}} (\Omega - 1)^{n_{\text{precipitation}}}$,
 - which is depended on the **calcite saturation state** $\Omega = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K_{\text{sp}}}$ 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

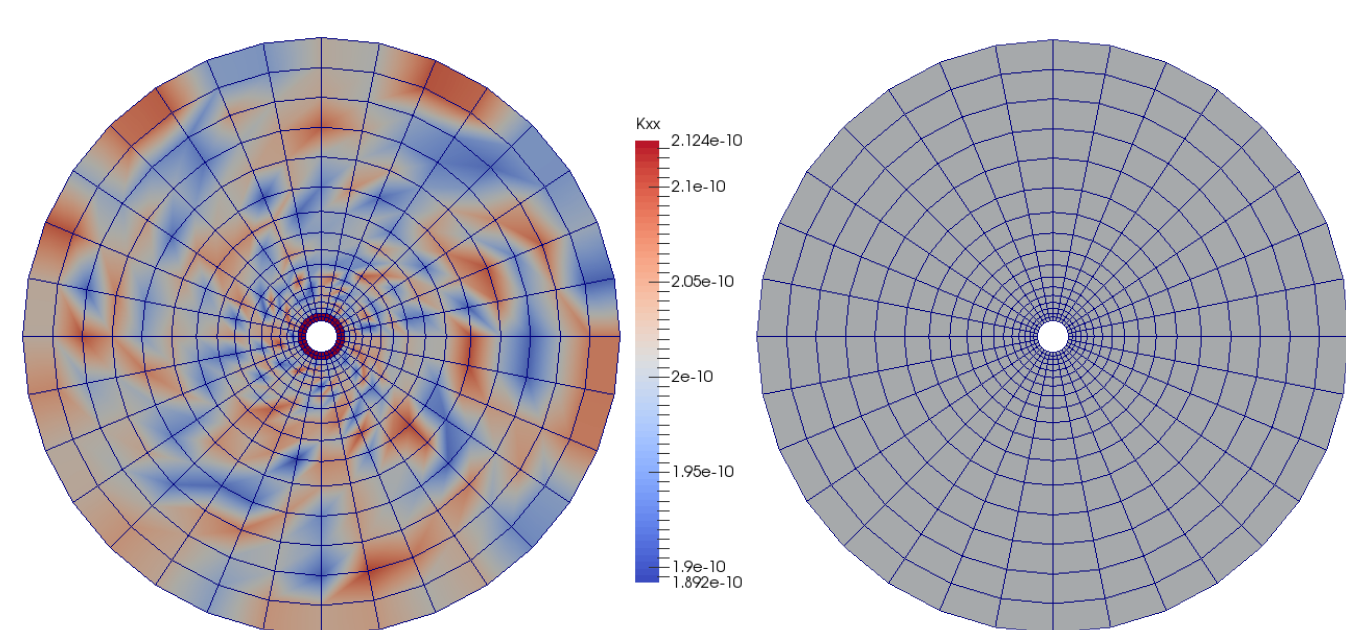


Figure 2 : Heterogeneous and homogeneous permeability used to calculate a base error to compare with the error of the model simplifications.

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

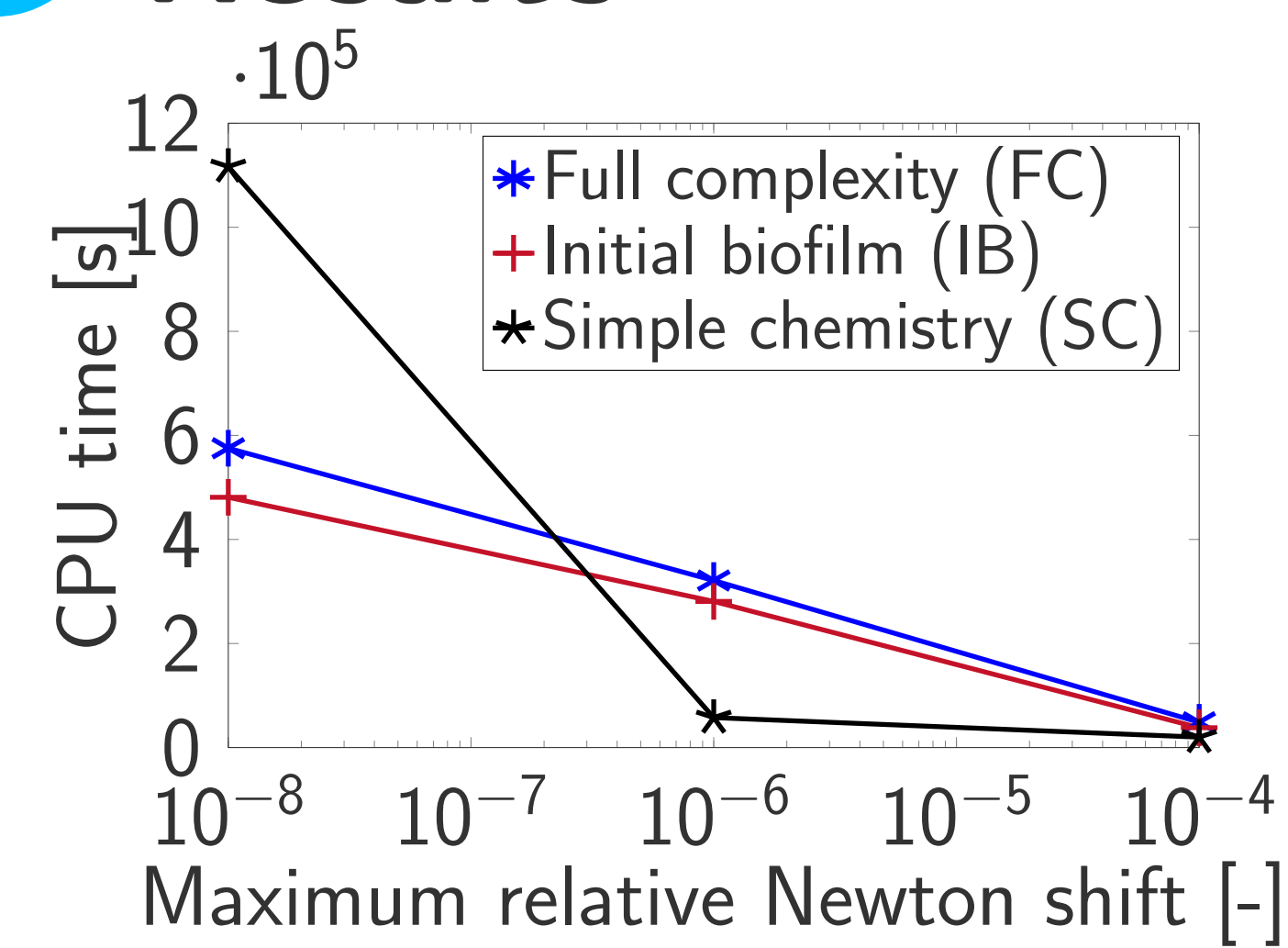


Figure 3 : CPU times for simplified models for various Newton tolerances.

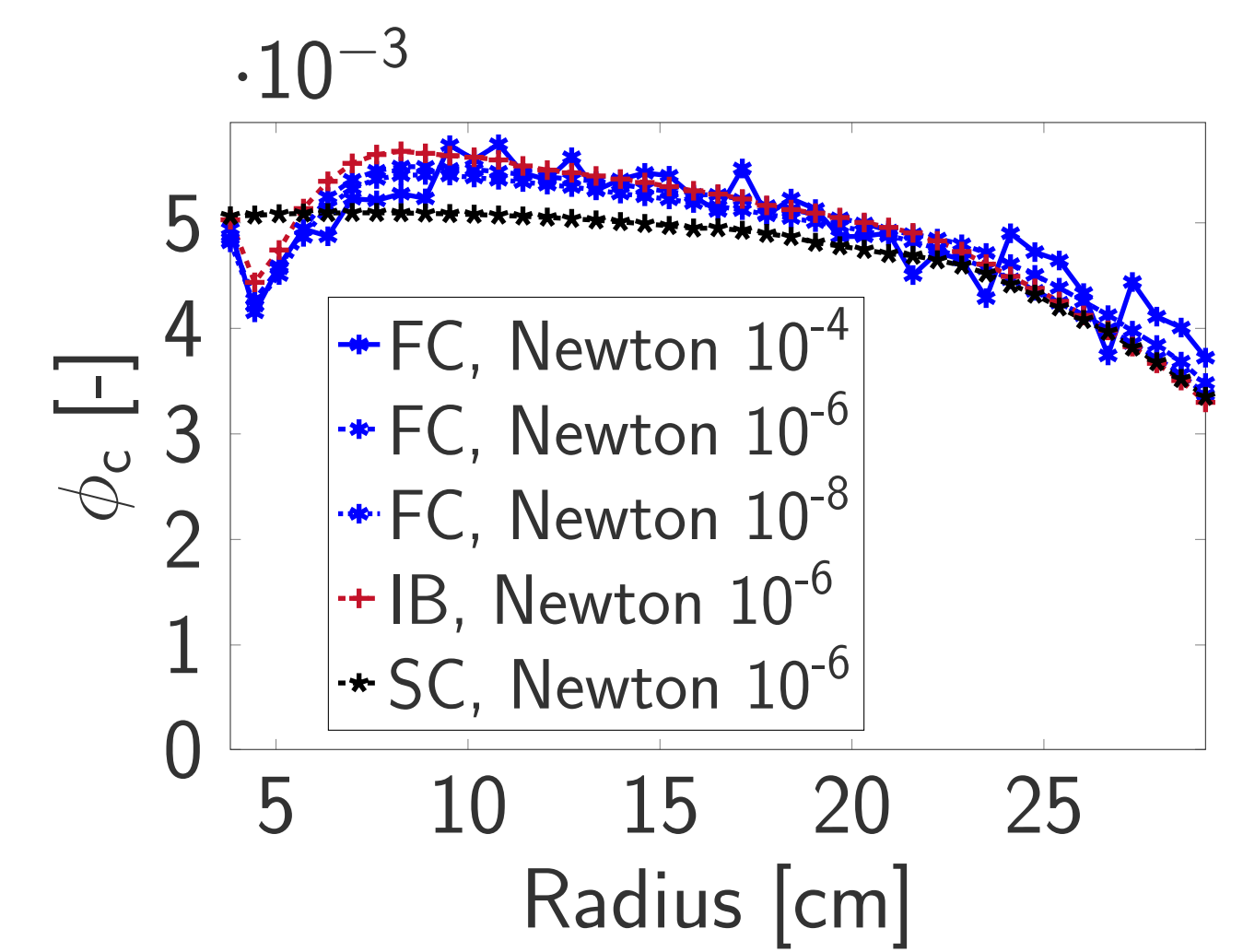


Figure 4 : Predictions of precipitated calcite after model simplifications.

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 NH₄⁺**, as the geochemistry is neglected in this setup.

Literature

- 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.
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