

Finding a balance between accuracy and effort for modeling biomineralization

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. (2013).

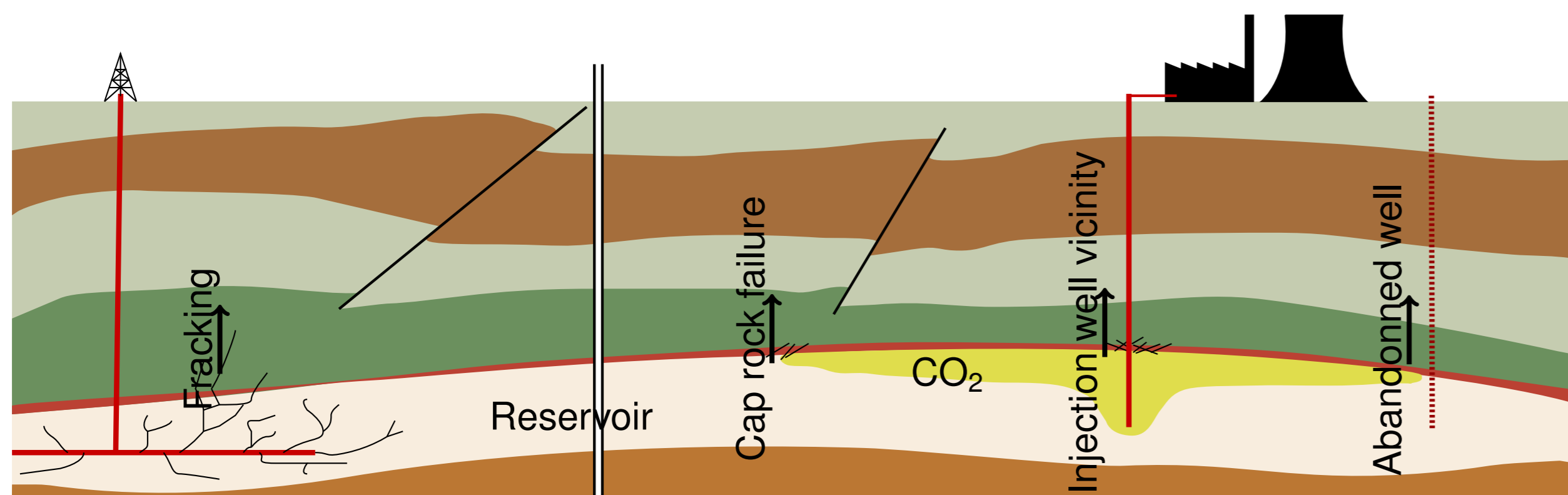


Figure 1 : Potential application sites of MICP as a sealing technology in the subsurface.

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**.

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

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

Relevant processes

Several bio- and geo-chemical processes, in combination with solute transport, are important for MICP:

- 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**:



$r_{\text{urea}} = k_{\text{urease}} k_{\text{ub}} \rho_{\text{biofilm}} \phi_{\text{biofilm}} \frac{m_{\text{urea}}}{m_{\text{urea}} + K_{\text{urea}}}$

- influence of NH_3 on the pH: $\text{NH}_3 + \text{H}^+ \leftrightarrow \text{NH}_4^+ \Rightarrow$ 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. (2015b).

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

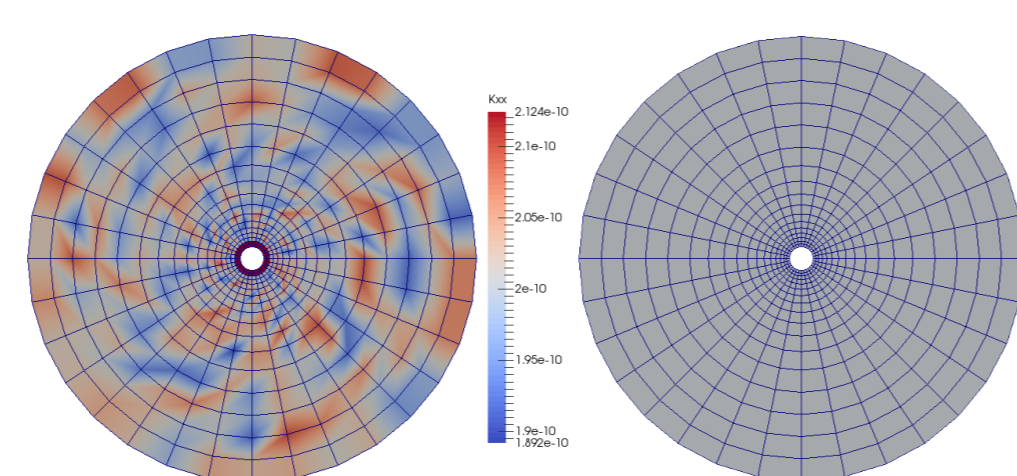


Figure 2 : Heterogeneous and homogeneous permeability used to calculate a base error to compare with the error of the model simplifications.



Approaches

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** (Hommel et al., 2015a), 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 van Wijngaarden et al. (2013), $r_{\text{prec}} = r_{\text{urea}}$. This model has the full set of unknowns.

Sequential calculation

In the sequential approach, the calculations and balance equations are split into reaction and transport. Thus, solid phases can be eliminated from the system of equations of the transport, which is expensive to solve. The splitted set of equations is solved non-iteratively.

Results

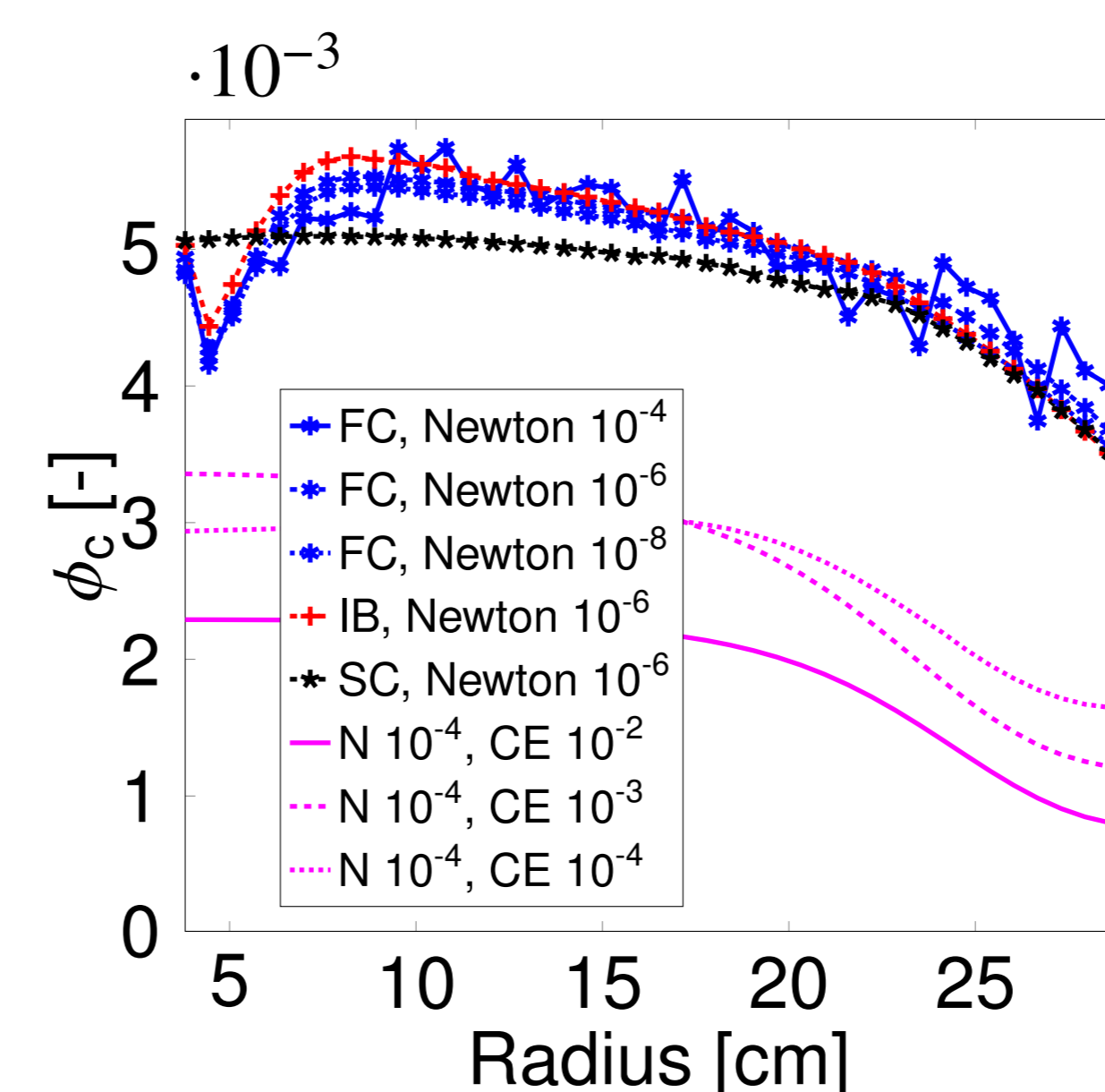


Figure 3 : Predictions of precipitated calcite after model simplifications or using the sequential approach.

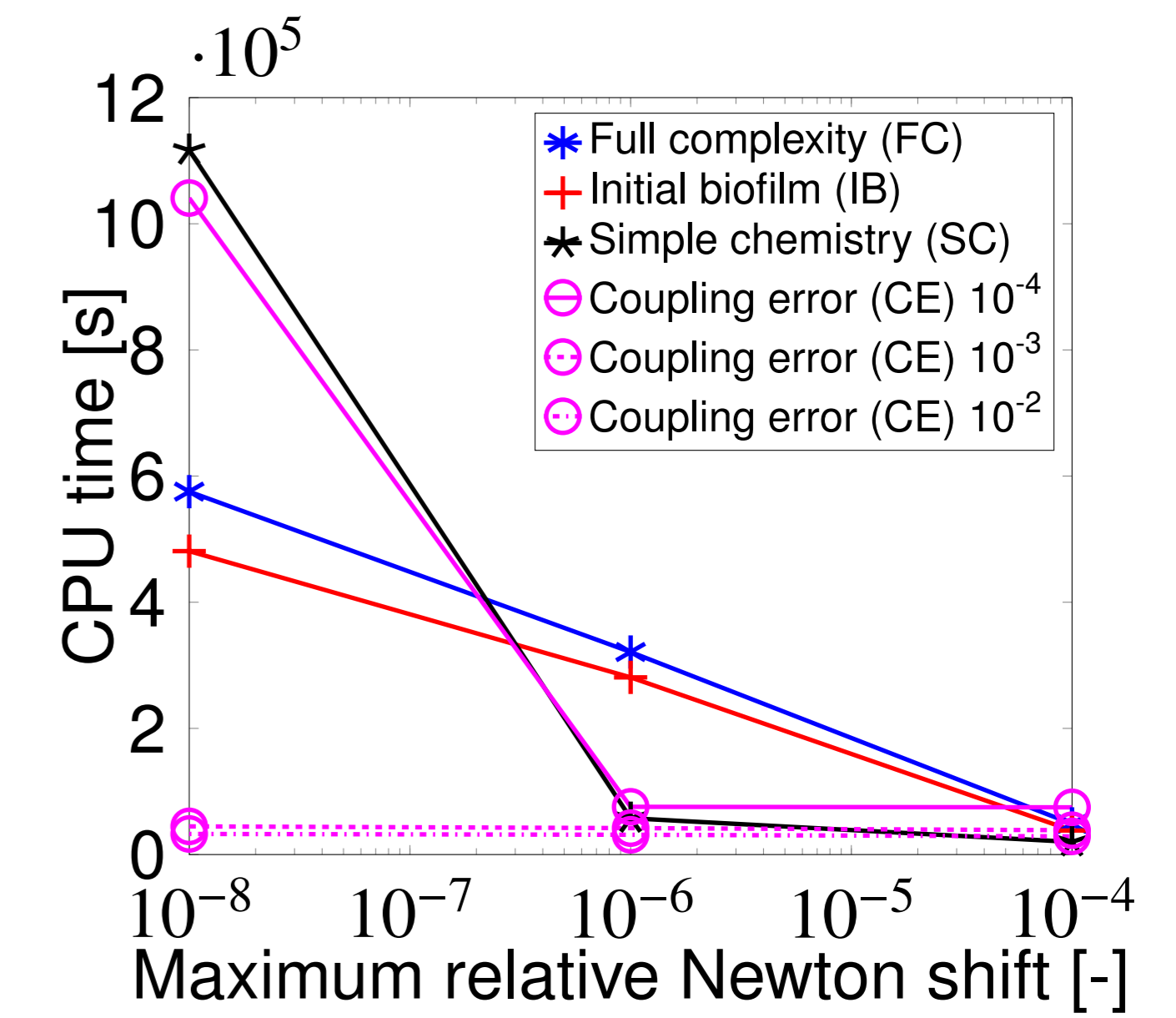


Figure 4 : CPU times for simplified models and sequential calculations for various Newton tolerances.

Table 1 : Comparison of simplified and sequential models. Reference error homogeneous to heterogeneous: 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
CE 10 ⁻² , N 10 ⁻⁴	2883 s	0.0770	327	12.28
CE 10 ⁻² , N 10 ⁻⁶	3136 s	0.0770	409	12.33
CE 10 ⁻⁴ , N 10 ⁻⁴	7486 s	0.0568	893	11.21

- The non-iterative sequential approach does not predict the results well.
- **Relaxing the Newton convergence criterion is a simple but effective measure to reduce CPU time.**
- For the given setup, the **simple chemistry model (at N 10⁻⁶) is comparable** to relaxing the Newton convergence criterion.

Literature

- J. Hommel, E. G. Lauchnor, R. Gerlach, A. B. Cunningham, Ebigbo, R. Helmig, and Class H. Investigating the influence of the initial biomass distribution and injection strategies on biofilm-mediated calcite precipitation in porous media. *Transport in Porous Media*, submitted, 2015a.
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- A. J. Phillips, R. Gerlach, E. G. Lauchnor, A. C. Mitchell, A. B. Cunningham, and L. H. Spangler. Engineered applications of ureolytic biomineralization: a review. *Biofouling*, 29(6):715–733, January 2013. doi: 10.1080/08927014.2013.796550.
- W. K. van Wijngaarden, F. J. Vermolen, G. A. M. Meurs, and C. Vuijk. A mathematical model for Biogrout. *Computational Geosciences*, 17(3):463–478, 2013. doi: 10.1007/s10596-012-9316-0.