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]. 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.  

\[
\text{solid phases} \frac{\partial}{\partial t} (\phi_i \rho_i) = q_{\text{reactions}}^i
\]

solutes:  

\[
\sum_i \frac{\partial}{\partial t} (\rho_i \phi_i x_i^S \phi_i) + \nabla \cdot (\rho_i \phi_i x_i^S \nabla \phi_i) = q_{\text{reactions}}^i
\]

Relevant processes

- two-phase multi-component flow
- processes determining the distribution of biomass:
  - growth: \( \alpha_{\text{biofilm}} = \beta \text{ Phosphate Uptake} \)
  - decay: \( \alpha_{\text{biofilm}} = \beta \text{ Phosphate Uptake} \)
  - attachment: \( \alpha_{\text{biofilm}} = (\alpha_S \phi_i x_i^S) \phi \text{ Chemisorption} \)
  - detachment: \( \alpha_{\text{biofilm}} = (\alpha_S \phi_i x_i^S) \phi \text{ Detachment} \)
- (bio-) chemical reactions:
  - microbially catalyzed ureolysis: \( \text{CO(NH}_2\text{)}_2 + 2 \text{H}_2\text{O} \xrightarrow{\text{ur} \text{ase}} 2 \text{NH}_3 + \text{H}_2\text{CO}_3 \)
  - influence of \( \text{NH}_3 \) on the pH: \( \text{NH}_3 + \text{H}^+ \leftrightarrow \text{NH}_4^+ \), increase in pH
  - precipitation (and dissolution) of calcite: \( \text{Ca}^{2+} + \text{CO}_3^{2-} \leftrightarrow \text{CaCO}_3 \downarrow \)
  - which is depended on the calcite saturation state \( \Omega = \frac{[\text{Ca}^{2+}][\text{CO}_3^{2-}]}{K_{sp}} \) and the water-solid surface area \( A_{\text{ss}} \)
  - clogging: \( \phi = \phi_0 - \phi_{\text{calcite}} - \phi_{\text{biofilm}} \Rightarrow K = K_0 \left( \frac{\phi_0}{\phi} \right)^3 \)

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

Results

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], \( \rho_{\text{biofilm}} = \rho_{\text{biofilm}} \). This model has the full set of unknowns, but the geochemistry is neglected.

Model simplification

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

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

<table>
<thead>
<tr>
<th>Model</th>
<th>CPU time</th>
<th>Error Newton it. Lin. it. / N. it</th>
</tr>
</thead>
<tbody>
<tr>
<td>FC, N 10⁻⁴</td>
<td>32110 s</td>
<td>0.0025 4971 15.15</td>
</tr>
<tr>
<td>FC, N 10⁻⁴</td>
<td>4861 s</td>
<td>0.0065 776 6.57</td>
</tr>
<tr>
<td>SC, N 10⁻⁴</td>
<td>5758 s</td>
<td>0.0070 1094 14.90</td>
</tr>
<tr>
<td>SC, N 10⁻⁴</td>
<td>2001 s</td>
<td>0.0104 396 13.14</td>
</tr>
<tr>
<td>IB, N 10⁻⁴</td>
<td>28098 s</td>
<td>0.0040 5053 14.9</td>
</tr>
</tbody>
</table>

- 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 10⁻⁴) 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