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,

\[
\text{solutes: } \sum_{\alpha} \left[ \frac{\partial}{\partial t} \left( \phi \rho_{\alpha} \right) \right] + \nabla \cdot \left( \phi \rho_{\alpha} \mathbf{v}_{\alpha} \right) - \nabla \cdot \left( \rho_{\alpha} \mathbf{D}_{\alpha} \nabla \phi \right) = q_{\text{reactions}}
\]

Relevant processes
- two-phase multi-component flow
- processes determining the distribution of biomass: growth, decay, attachment, detachment, (bio-) chemical reactions:
- microbially catalyzed ureolysis: CO(NH\textsubscript{2})\textsubscript{2} + 2H\textsubscript{2}O $\rightarrow$ 2NH\textsubscript{3} + H\textsubscript{2}CO\textsubscript{3};
- influence of NH\textsubscript{3} on the pH: NH\textsubscript{3} + H\textsuperscript{+} $\rightarrow$ NH\textsubscript{4}\textsuperscript{+} $\rightarrow$ increase in pH,
- precipitation and dissolution of calcite: Ca\textsuperscript{2+} + CO\textsubscript{3}\textsuperscript{2–} $\rightarrow$ CaCO\textsubscript{3};
- which is dependet on the calcite saturation state: $K = K_{\text{IC}} \left( \frac{\phi_{\text{calcite}} - \phi_{\text{biofilm}}}{\phi_{\text{calcite}} - \phi_{\text{biofilm}}} \right)^3$.

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 homogenity to the model simplifications

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

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], $r_{\text{calcite}} = r_{\text{biofilm}}$. This model has the full set of unknowns, but the geochemistry is neglected.

Figure 4: Predictions of precipitated calcite after model simplifications.

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 int. Lin. it. / N. it</th>
</tr>
</thead>
<tbody>
<tr>
<td>FC, N 10\textsuperscript{−4}</td>
<td>32110 s</td>
<td>0.0025</td>
</tr>
<tr>
<td>FC, N 10\textsuperscript{−6}</td>
<td>4861 s</td>
<td>0.0065</td>
</tr>
<tr>
<td>SC, N 10\textsuperscript{−4}</td>
<td>5758 s</td>
<td>0.0070</td>
</tr>
<tr>
<td>SC, N 10\textsuperscript{−6}</td>
<td>2001 s</td>
<td>0.0104</td>
</tr>
<tr>
<td>IB, N 10\textsuperscript{−6}</td>
<td>28089 s</td>
<td>0.0040</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\textsuperscript{−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\textsuperscript{+}, Cl\textsuperscript{−}, and NH\textsubscript{3}\textsuperscript{2–}, as the geochemistry is neglected in this setup.

Literature

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www.hydrosys.uni-stuttgart.de