Motivation

With increasing intensity of subsurface use, ensuring separation between different layers with competitive uses becomes more and more important. The risk of polluting upper layers, e.g. used for drinking water production, by applications such as CO₂ storage in the subsurface or fracking could be reduced with sealing technologies like microbially induced calcite precipitation (MICP). Other applications of MICP are discussed in [5].

Model concept

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

\[ \frac{\partial}{\partial t} (\rho \phi) + \nabla \cdot (\rho \phi \mathbf{v}) = q_{\text{reactions}} \]

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: \( r_{\text{growth}} = \mu \cdot \text{Prec} \cdot \phi_{\text{biom}} \cdot C_{\text{NH}_4} \)
  - decay: \( r_{\text{decay}} = k_{\text{decay}} \cdot \phi_{\text{biom}} \cdot C_{\text{NH}_4} \)
  - attachment: \( r_{\text{attachment}} = k_{\text{attachment}} \cdot (S \cdot \phi - \phi_{\text{attachment}}) \cdot C_{\text{NH}_4} \)
  - detachment: \( r_{\text{detachment}} = k_{\text{attachment}} \cdot (S \cdot \phi - \phi_{\text{attachment}}) \)
  - (bio-) chemical reactions:
    - microbially catalyzed ureolysis: \( \text{CO(NH}_2)_2 + 2 \text{H}_2 \text{O} \rightarrow \text{2NH}_3 + \text{CO}_2 \)
    - influence of NH₃ on the pH: \( \text{NH}_3 + \text{H}^+ \rightarrow \text{NH}_4^+ \rightarrow \text{increase in pH} \)
    - precipitation (and dissolution) of calcite: \( \text{Ca}^{2+} + \text{CO}_3^{2-} \rightarrow \text{CaCO}_3 \cdot \)

which is dependent on the calcite saturation state \( \xi = (\text{Ca}^{2+} \cdot \text{CO}_3^{2-}) \) and the water-solid surface area \( \phi_{\text{wss}} \).

clogging: \( \phi = \phi_{\text{wss}} - \phi_{\text{attachment}} \rightarrow K = K_0 \left( \phi_{\text{wss}} - \phi_{\text{attachment}} \right)^{n} \)

Permeability

As updating \( \phi_{\text{wss}} \) is not sufficient to match experimentally observed permeability reductions [3], a shape parameter \( S = f(\phi_{\text{wss}}) \) is included to account for the additional change in pore geometry attributed to biofilm presence.

\[ K = K_0 \left( \frac{\phi_{\text{wss}}}{\phi_{\text{wss}} - \phi_{\text{attachment}}} \right)^{n} \]

Ureolysis

In recent kinetic studies on the ureolysis by Sporosarcina pasteurii, CO(NH₃)₂ + 2 H₂O \u2192 \text{2NH}_3 + \text{CO}_2 \text{H}_3 \text{O}

kinetic parameters were determined at Montana State University. The improved knowledge is updated into the numerical model replacing the previously used ureolysis rate equation [1] which was determined for pure, isolated jack bean urease by [2].

\[ r_{\text{urea,old}} = k_{\text{urea,old}} \left( \frac{\phi_{\text{biom}}}{\phi_{\text{biom}} + K_{\text{NH}_4}} \right)^{n} \] \( \text{urease} \)

The new rate equation according to experiments with whole cells of S. pasteurii, as used in MICP applications, is independent of NH₃ and H⁺ concentrations:

\[ r_{\text{urea,new}} = k_{\text{urea,new}} \left( \frac{\phi_{\text{biom}}}{\phi_{\text{biom}} + K_{\text{NH}_4}} \right)^{n} \]

The improved implementation of ureolysis causes a need to refit the model, since the updated kinetic parameters are significantly different from the previously used ones. Instead of trial-and-error methods, this refit is conducted using inverse modeling. Fitted parameters are the biofilm density \( \phi_{\text{bio}} \), the attachment coefficient of bacteria to biofilm \( k_{\text{attachment}} \), and the attachment coefficient of bacteria to arbitrary solid surfaces \( k_{\text{attachment}} \).

Literature


