Estimation of uncertain parameters to improve modeling of Mirobially Induced Calcite Precipitation

Johannes Hommel†, Ellen Lauchnor‡, Alfred B. Cunningham*, Rainer Helmsg*, Anozie Ebigo‡, Holger Class*

*IWS, University of Stuttgart; ‡CBE, Montana State University; GGE, RWTH Aachen University
EGU General Assembly, May 22nd 2014

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 fracturing could be reduced with sealing technologies like microbiologically induced calcite precipitation (MICP). Other applications of MICP are discussed in [3].

MICP has several advantages:

⇒ low viscosity ⇒ reduced injection pressure and increased radial extent,
⇒ catalyzed reactions in the medium ⇒ plugging is dependent on injection scheme ⇒ porosity and permeability distribution can be engineered.
⇒ MICP is a promising sealing technology that needs further research before it can be meaningfully applied on field scale.

Model concept

The REV-scale MICP model includes reactive two-phase multi-component transport:

\[
\frac{\partial}{\partial t} (\rho_{\text{w}} \phi_{\text{w}} c) + \nabla \cdot (\rho_{\text{w}} \phi_{\text{w}} \mathbf{v}_\text{w}) - \nabla \cdot (\rho_{\text{w}} D_{\text{pmw}} \nabla c) = q_{\text{reactions}}
\]

where \(q_{\text{reactions}}\) represents the biofilm density \(\rho_{\text{biofilm}}\), the attachment coefficient of bacteria to biofilm \(a_{1,2}\), and the attachment coefficient of bacteria to arbitrary solid surfaces \(a_{2,2}\).

Relevant processes

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

⇒ processes determining the distribution of biomass:
  - growth: \(r_{\text{growth}} = \mu \text{F} \text{euc}\phi_{\text{biofilm}}\)
  - decay: \(r_{\text{decay}} = \phi_{\text{biofilm}} \mu_{\text{biofilm}}\)
  - attachment: \(r_{\text{attachment}} = (s_{\text{u}} \phi_{\text{biofilm}} + c_{\text{u}}) S_{\text{w}} = \phi_{\text{biofilm}}\)
  - detachment: \(r_{\text{detachment}} = c_{\text{d}} (S_{\text{w}} \phi_{\text{biofilm}})^{0.5} + c_{\text{d}} \mu_{\text{biofilm}}\)
⇒ (bio-) chemical reactions:
  - microbiologically catalyzed ureolysis: \(\text{CO(NH}_2\text{)}_2 + 2 \text{H}_2\text{O} \rightarrow 2 \text{NH}_3 + \text{H}_2\text{CO}_3\)
  - influence of NH4 on the pH: \(\text{NH}_4^+ + \text{H}_2\text{O} \rightarrow \text{NH}_3 + \text{H}_3\text{O}^+\)
  - precipitation (and dissolution) of calcite: \(\text{Ca}^{2+} + \text{CO}_3^{2-} \rightarrow \text{CaCO}_3\)
⇒ sensitivity analysis of the model with respect to the fitted parameters.

Model improvement

In recent studies on the main driving force of MICP, the microbial ureolysis, \(\text{CO(NH}_2\text{)}_2 + 2 \text{H}_2\text{O} \rightarrow 2 \text{NH}_3 + \text{H}_2\text{CO}_3\)
kinetic parameters were determined by batch kinetic studies of Sporosarcina pasteurii performed at Montana State University. The improved knowledge made it necessary to update the implementation of ureolysis in the numerical model. Contrary to the previously used ureolysis rate equation as implemented in [1] which was determined for pure, isolated jack bean urease by [2],

\[
r_{\text{urea, ol}} = \frac{k_{\text{urease}}}{1 + \frac{K_{\text{urea}}}{c_{\text{urea}}}} (\rho_{\text{biofilm}} \phi_{\text{biofilm}}) \frac{\text{urea}}{\text{biofilm}}
\]

the new rate equation according to experiments with whole cells of the bacteria used in MICP applications, Sporosarcina pasteurii, is independent of the concentrations of NH4 and H+:

\[
r_{\text{urea, new}} = k_{\text{urease}, \text{new}} \text{new} \text{biofilm} \text{biofilm}
\]

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.

Inverse Modelling

In inverse modeling, the goal is to estimate unknown or uncertain input parameters. This estimation is based on the minimization of an objective function, which compares simulation results and observations. Additionally to the best fit parameter values, inverse modeling provides statistical and sensitivity analysis of the model with respect to the fitted parameters.

Results

The fitted parameters are the biofilm density \(\rho_{\text{biofilm}}\), the attachment coefficient of bacteria to biofilm \(c_{1,2}\), and the attachment coefficient of bacteria to arbitrary solid surfaces \(c_{2,2}\).

![Comparison of measured concentrations at 0.4 m distance from the inlet to two simulation results obtained with different sets of parameters, which were both fitted to experimental data obtained in sand-filled column studies of MICP by Sporosarcina pasteurii conducted at Montana State University.](image)

Literature