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

International Research Training Group nupus

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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 CO_2 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 [3].

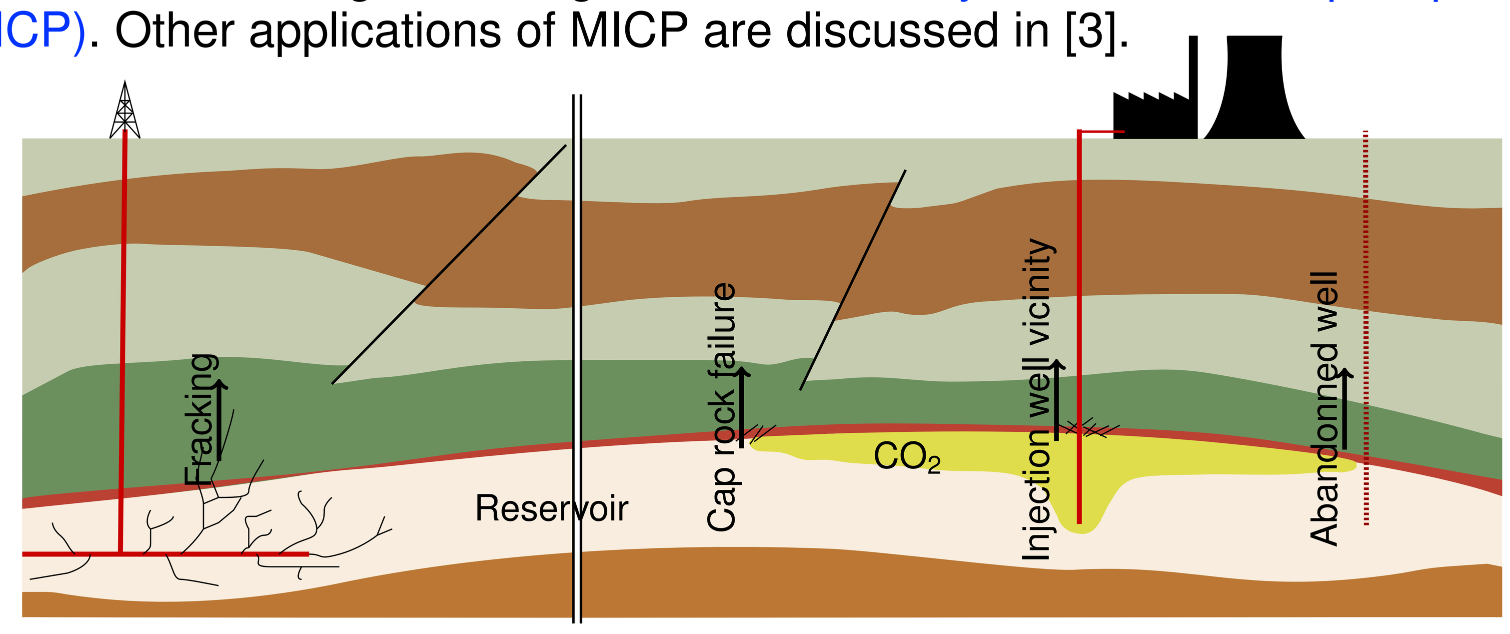

Figure 1: *Potential application sites of MICP as a sealing technology in the subsurface.*

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.

$$\sum_{\alpha}\left[\frac{\partial}{\partial t}(\phi\rho_\alpha x_\alpha^\kappa S_\alpha) + \nabla\cdot(\rho_\alpha x_\alpha^\kappa \mathbf{v}_\alpha) - \nabla\cdot\left(\rho_\alpha \mathbf{D}_{\mathrm{pm},\alpha}\nabla x_\alpha^\kappa\right)\right] = q^\kappa_{\mathrm{reactions}}$$

$$\frac{\partial}{\partial t}(\phi_\lambda\rho_\lambda) = q^\lambda_{\mathrm{reactions}}$$

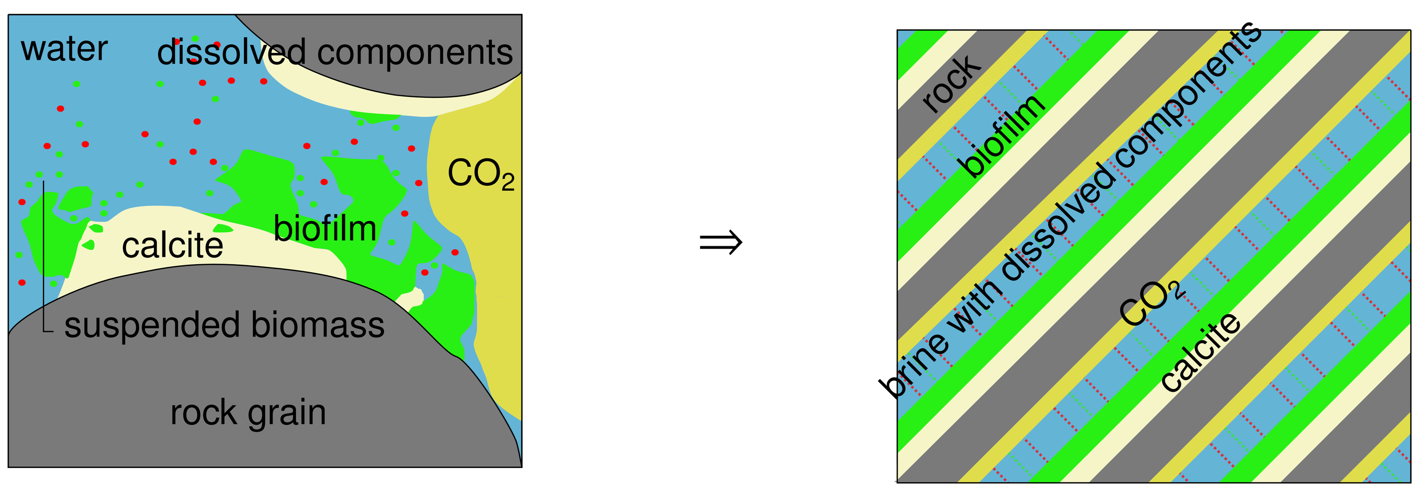

Figure 2: *Model relevant phases and distribution of components in the phases at pore scale and REV-scale, modified from [1].*

Relevant processes

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

- processes determining the distribution of biomass:
  - growth: $r_{\mathrm{growth}} = \mu\,\rho_{\mathrm{biofilm}}\,\phi_{\mathrm{biofilm}}\,\frac{C_w^{O_2}}{C_w^{O_2}+K_{O_2}}\,\frac{C_w^{\mathrm{substrate}}}{C_w^{\mathrm{substrate}}+K_{\mathrm{substrate}}}$,
  - decay: $r_{\mathrm{decay}} = k_{\mathrm{decay}}\,\rho_{\mathrm{biofilm}}\,\phi_{\mathrm{biofilm}}$,
  - attachment: $r_{\mathrm{attachment}} = (c_{a,1}\,\phi_{\mathrm{biofilm}} + c_{a,2})\,S_w\,\phi\,C_w^{\mathrm{bacteria}}$,
  - detachment: $r_{\mathrm{detachment}} = c_{d,1}\,(S_w\,\phi\,|\nabla p_w|)^{0.58} + c_{d,2}\,\mu$,
- (bio-) chemical reactions:
  - microbially catalyzed ureolysis: $CO(NH_2)_2 + 2\,H_2O \xrightarrow{\mathrm{urease}} 2\,NH_3 + H_2CO_3$,
  - influence of NH_3 on the pH: $NH_3 + H^+ \leftrightarrow NH_4^+$ ⇒ increase in pH,
  - precipitation (and dissolution) of calcite: $Ca^{2+} + CO_3^{2-} \leftrightarrow CaCO_3\downarrow$,

    $r_{\mathrm{precipitation}} = k_{\mathrm{precipitation}}\,A_{\mathrm{sw}}\,(\Omega-1)^{n_{\mathrm{precipitation}}}$,

    which is depended on the calcite saturation state $\Omega = \frac{[Ca^{2+}][CO_3^{2-}]}{K_{\mathrm{sp}}}$ and the water-solid surface Area A_{sw}.
  - clogging: $\phi = \phi_0 - \phi_{\mathrm{calcite}} - \phi_{\mathrm{biofilm}} \Rightarrow K = K_0\left(\frac{\phi-\phi_{\mathrm{crit}}}{\phi_0-\phi_{\mathrm{crit}}}\right)^3$

DuMux — Simulations are performed using the open-source simulator DuMux.

DFG — Support of the German Research Foundation is gratefully acknowledged.

Link to this poster.

Model improvement

In recent studies on the main driving force of MICP, the microbial ureolysis,

$$CO(NH_2)_2 + 2\,H_2O \xrightarrow{\mathrm{urease}} 2\,NH_3 + H_2CO_3$$

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],

$$r_{\mathrm{urea,\,old}} = \frac{k_{\mathrm{urease}}}{1+\frac{m^{H^+}}{K_{\mathrm{eu},1}}+\frac{K_{\mathrm{eu},1}}{m^{H^+}}}\,k_{\mathrm{ub}}\left(\rho_{\mathrm{biofilm}}\,\phi_{\mathrm{biofilm}}\right)^{n_{\mathrm{ub}}}\,\frac{m^{\mathrm{urea}}}{m^{\mathrm{urea}}+K_{\mathrm{urea}}}\,\frac{K_{NH_4^+}}{m^{NH_4^+}+K_{NH_4^+}}$$

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 NH_4^+ and H^+:

$$r_{\mathrm{urea,\,new}} = k_{\mathrm{urease,\,new}}\,k_{\mathrm{ub,\,new}}\,\rho_{\mathrm{biofilm}}\,\phi_{\mathrm{biofilm}}\,\frac{m^{\mathrm{urea}}}{m^{\mathrm{urea}}+K_{\mathrm{urea,\,new}}}.$$

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 ρ_{biofilm}, the attachment coefficient of bacteria to biofilm $c_{a,1}$, and the attachment coefficient of bacteria to arbitrary solid surfaces $c_{a,2}$.

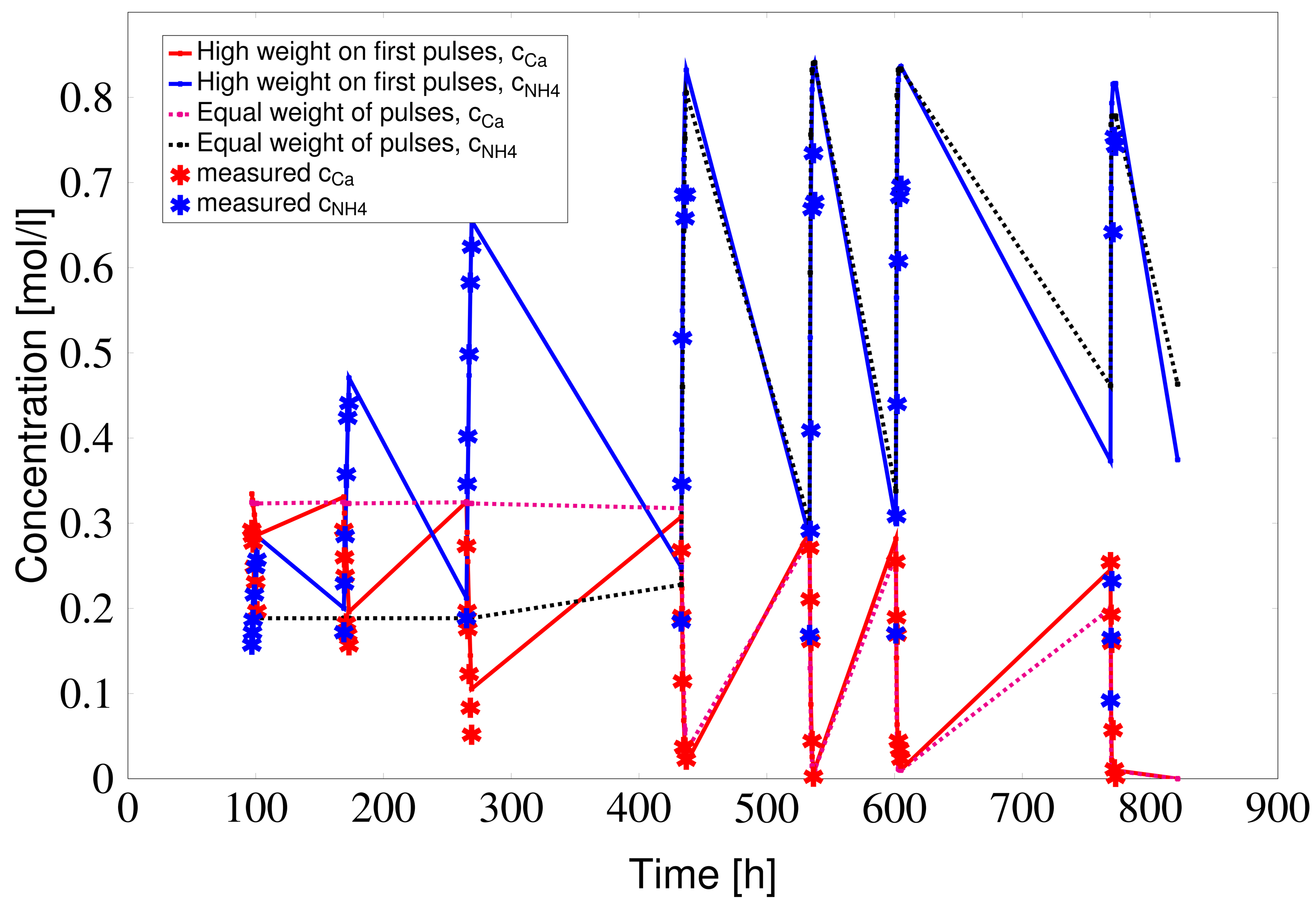

Figure 3: *Comparison of measured concentrations at 0.4 m distance from the inlet to two simulation results obtained with different sets of parameters, which were both fitted to experimental data obtained in sand-filled column studies of MICP by Sporosarcina pasteurii conducted at Montana State University.*

Literature

[1] Anozie Ebigbo, Adrienne J Phillips, Robin Gerlach, Rainer Helmig, Alfred B Cunningham, Holger Class, and Lee H Spangler. Darcy-scale modeling of microbially induced carbonate mineral precipitation in sand columns. *Water Resources Research*, 48(7):W07519, July 2012.

[2] Marcello Fidaleo, and Roberto Lavecchia. Kinetic study of enzymatic urea hydrolysis in the pH range 4-9. *Chemical and Biochemical Engineering Quarterly*, 17:311-318, 2003.

[3] Adrienne J Phillips, Robin Gerlach, Ellen Lauchnor, Andrew C Mitchell, Alfred B Cunningham, and Lee Spangler. Engineered applications of ureolytic biomineralization: a review. *Biofouling*, 29(6):715–733, January 2013.