Estimation of uncertain parameters of the biomineralization model by inverse modeling

International Research Training Group nupus

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NUPUS Meeting Freudenstadt, March 16-19th 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 for example 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 [2].

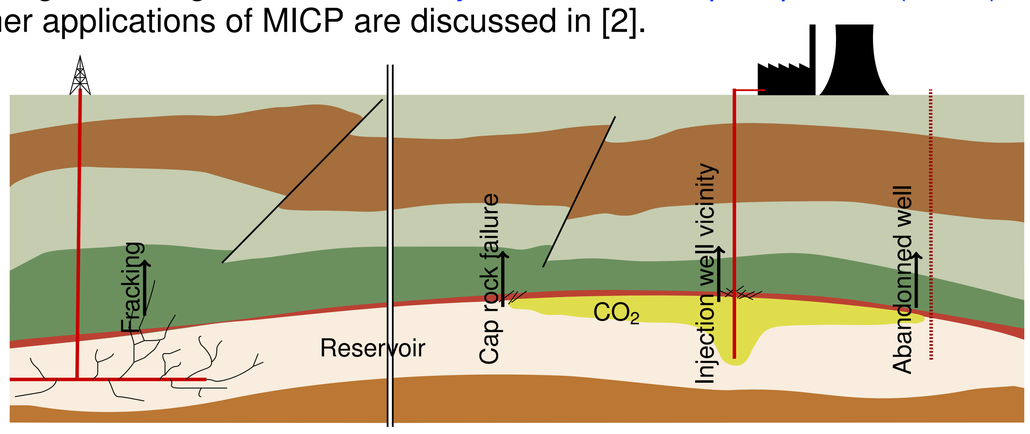

Figure 1: *Potential application sites of MICP as a sealing technology in the subsurface.*

Model concept

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

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

$$\frac{\partial}{\partial t}\left(\phi_{\lambda}\rho_{\lambda}\right)=q^{\lambda}_{\text{reactions}}$$

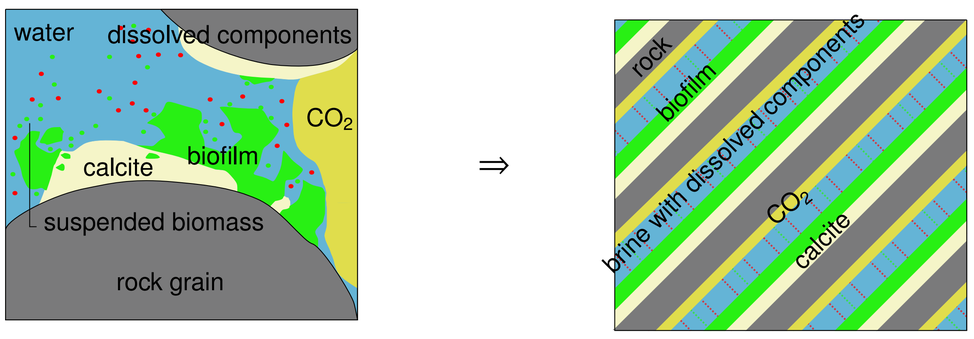

Figure 2: *Model relevant phases and distribution of components in the phases at pore scale and REV-scale, modified from [1].*

Model improvement

New findings on the main driving force of MICP, the microbial ureolysis

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

made it necessary to update the implementation of ureolysis in the numerical model. Contrary to the previously used ureolysis kinetic from [1],

$$r_{\text{urea, old}} = \frac{k_{\text{urease}}}{1+\frac{m^{\mathrm{H}^+}}{K_{\text{eu},1}}+\frac{K_{\text{eu},1}}{m^{\mathrm{H}^+}}}\,k_{\text{ub}}\,(\rho_{\text{f}}\phi_{\text{f}})^{n_{\text{ub}}}\,\frac{m^{\text{u}}}{m^{\text{u}}+K_{\text{u}}}\,\frac{K_{\mathrm{NH}_4^+}}{m^{\mathrm{NH}_4^+}+K_{\mathrm{NH}_4^+}}$$

the new kinetic is independent of the concentrations of NH_4^+ and H^+:

$$r_{\text{urea, new}} = k_{\text{urease}}\,k_{\text{ub}}\,(\rho_{\text{f}}\phi_{\text{f}})^{n_{\text{ub}}}\,\frac{m^{\text{u}}}{m^{\text{u}}+K_{\text{u}}}.$$

The improved implementation of ureolysis causes a need to refit the model. 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.

DuMu^x Simulations are performed using the open-source simulator DuMu^x.

DFG Support of the German Research Foundation is gratefully acknowledged.

Results

The fitted parameters are the biofilm density ρ_{f}, the attachment coefficient of bacteria to biofilm $c_{\text{a},1}$, and the attachment coefficient of bacteria to arbitrary solid surfaces $c_{\text{a},2}$. Additionally, since the urease content of the biofilm k_{ub} is also not well known, it is used as fourth fitting parameter in selected inverse model runs.

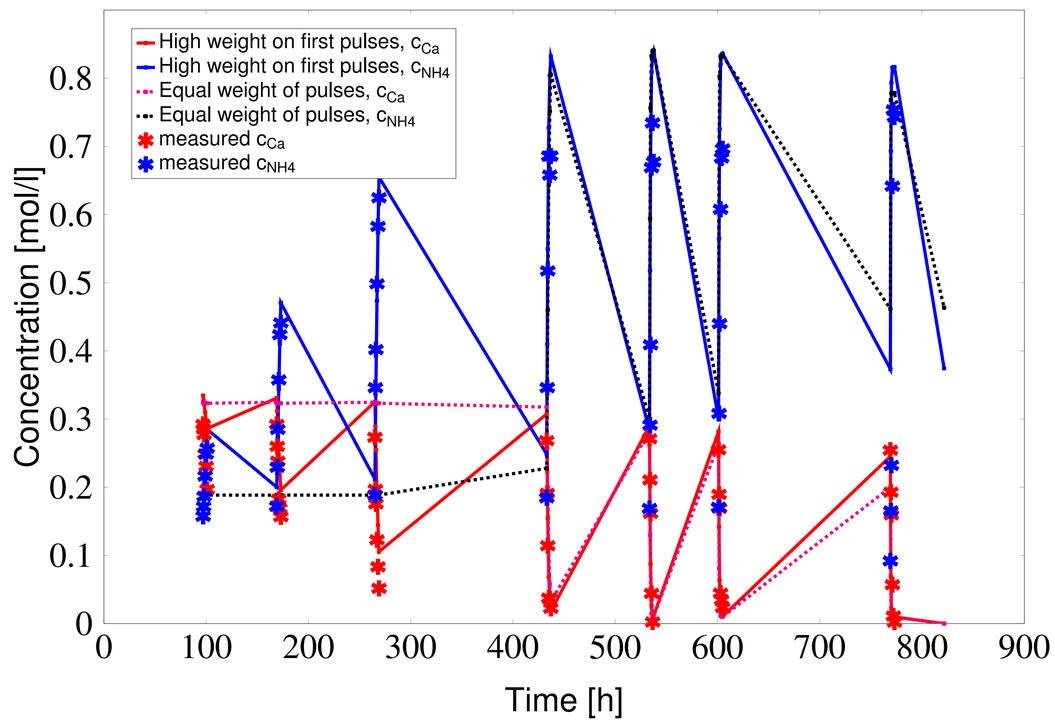

Figure 3: *Comparison of measured concentrations at 0.4 m distance from the inlet to two simulation results obtained with different sets of parameters, which were both fitted to column 9 data.*

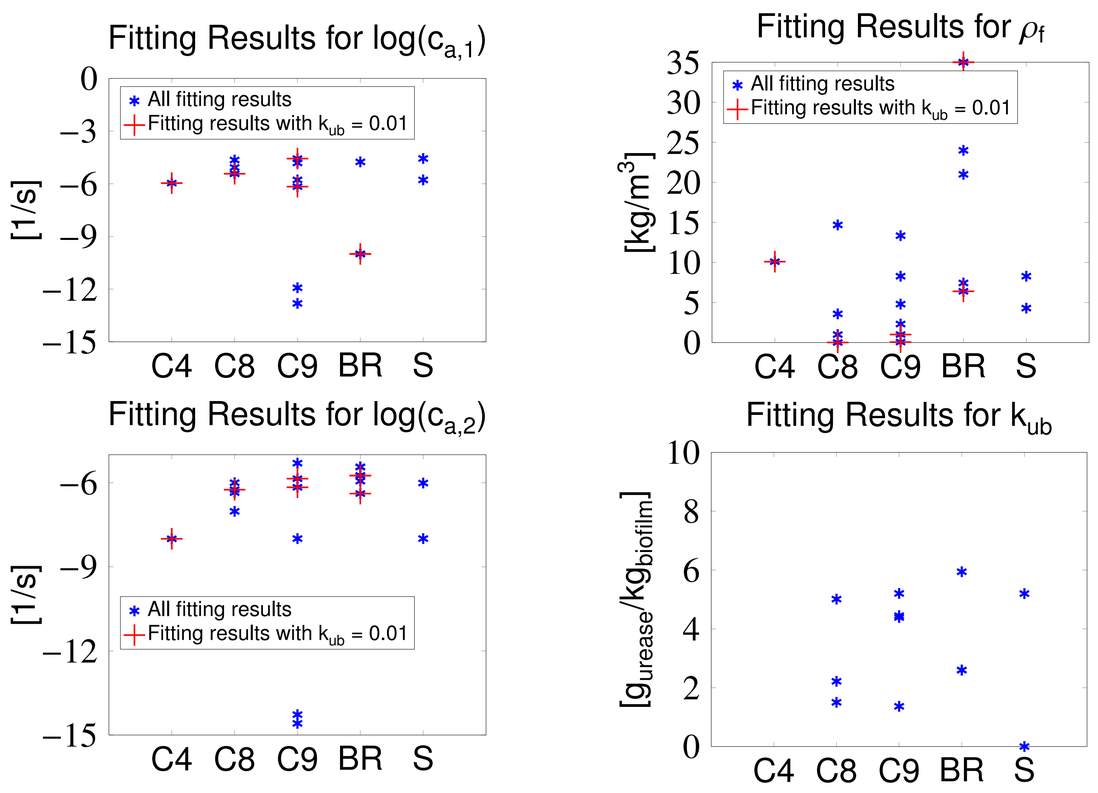

Figure 4: *Parameter values obtained by inverse modeling against different experimental data sets. The experiments C4, C8 and C9 are column experiments, BR is a 2D, radial flow experiment, and S is an inverse model setup in which C4, C9 and BR data was used for calibration.*

Summary

- There is no unique solution to the inverse MICP model.
- The obtained parameter values are dependent on the initial guesses and the weighting of the different experimental data sets used for calibration.
- Inverse modelling is a useful tool for estimating non-measurable parameters like the attachment coefficients of the MICP model.

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] 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):715–33, January 2013.