Improvements in Modeling Microbially Induced Calcite Precipitation as a Leakage Mitigation Technology

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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 [5].

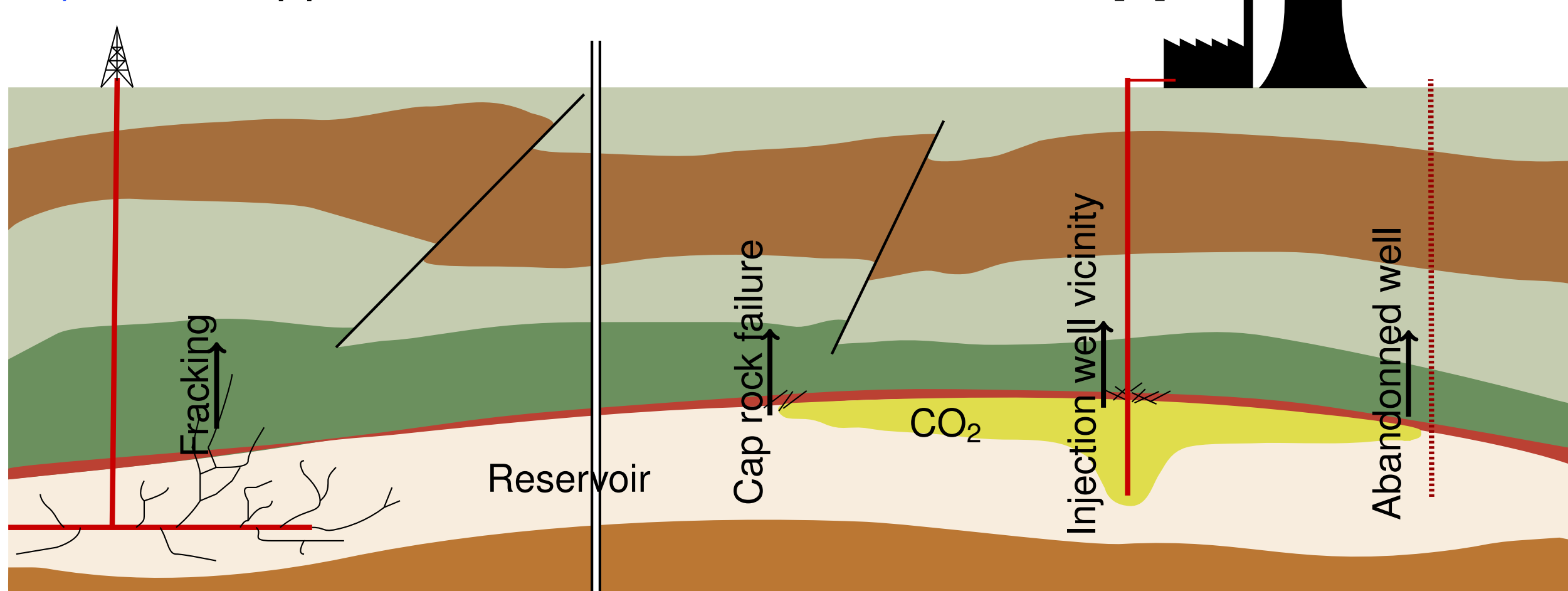Figure 1: Potential application sites of MICP as a sealing technology in the subsurface.

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.

Model concept

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

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

$$\sum_\alpha \left[\frac{\partial}{\partial t}(\phi \rho_\alpha x^\kappa_\alpha S_\alpha) + \nabla \cdot (\rho_\alpha x^\kappa_\alpha \mathbf{v}_\alpha) - \nabla \cdot \left(\rho_\alpha \mathbf{D}_{\text{pm},\alpha} \nabla x^\kappa_\alpha \right) \right] = q^\kappa_{\text{reactions}}$$
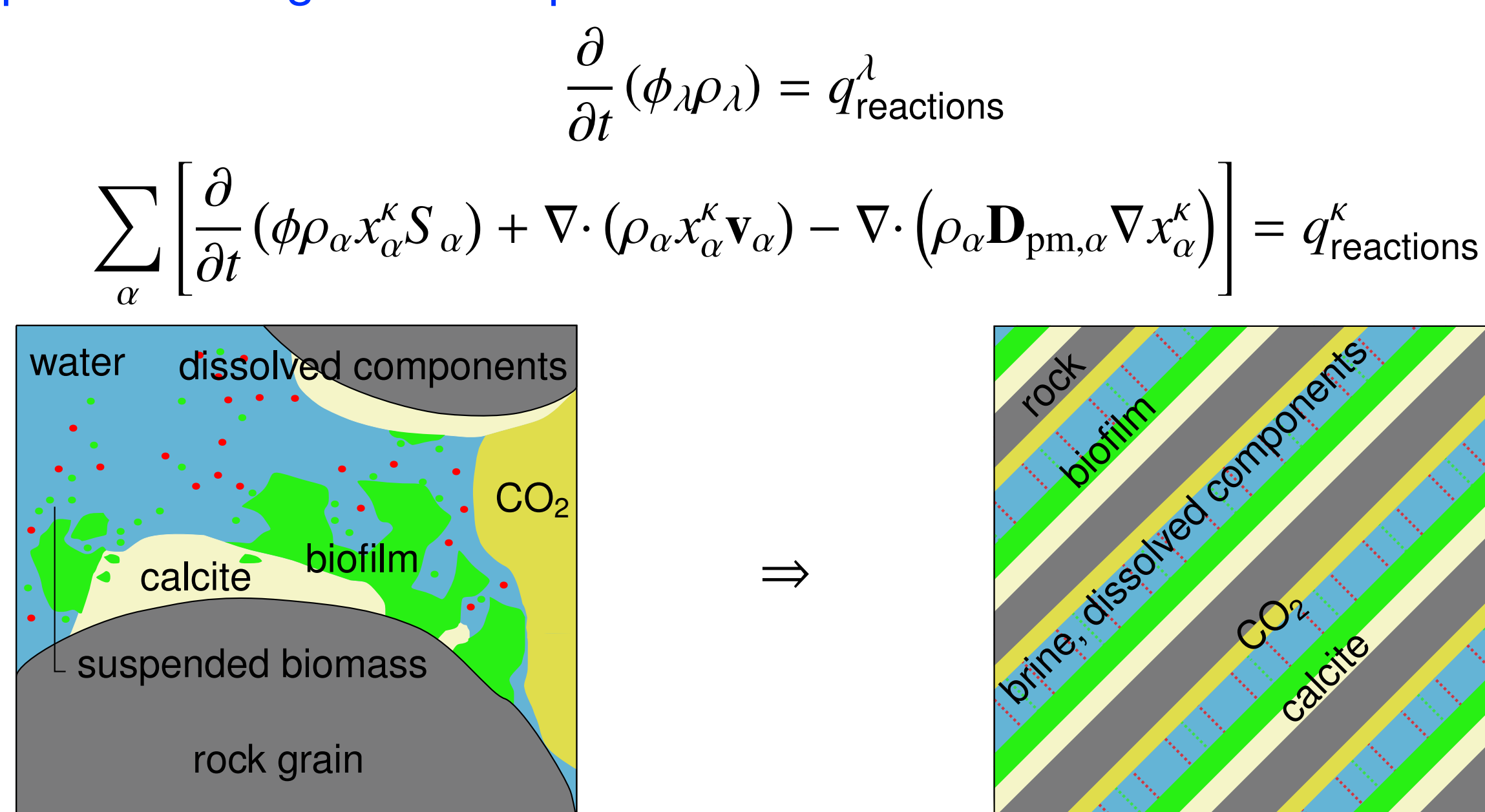
Figure 2: Model relevant phases and distribution of components in the phases at pore scale and REV-scale, modified from [1].

Relevant processes

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

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

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

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

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

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Link to this poster.

Model improvement

Permeability

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

$$K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}} \right)^3 \Rightarrow K = K_0 \left(\frac{\phi - \phi_{\text{crit}}}{\phi_0 - \phi_{\text{crit}}} \right)^n \cdot S$$
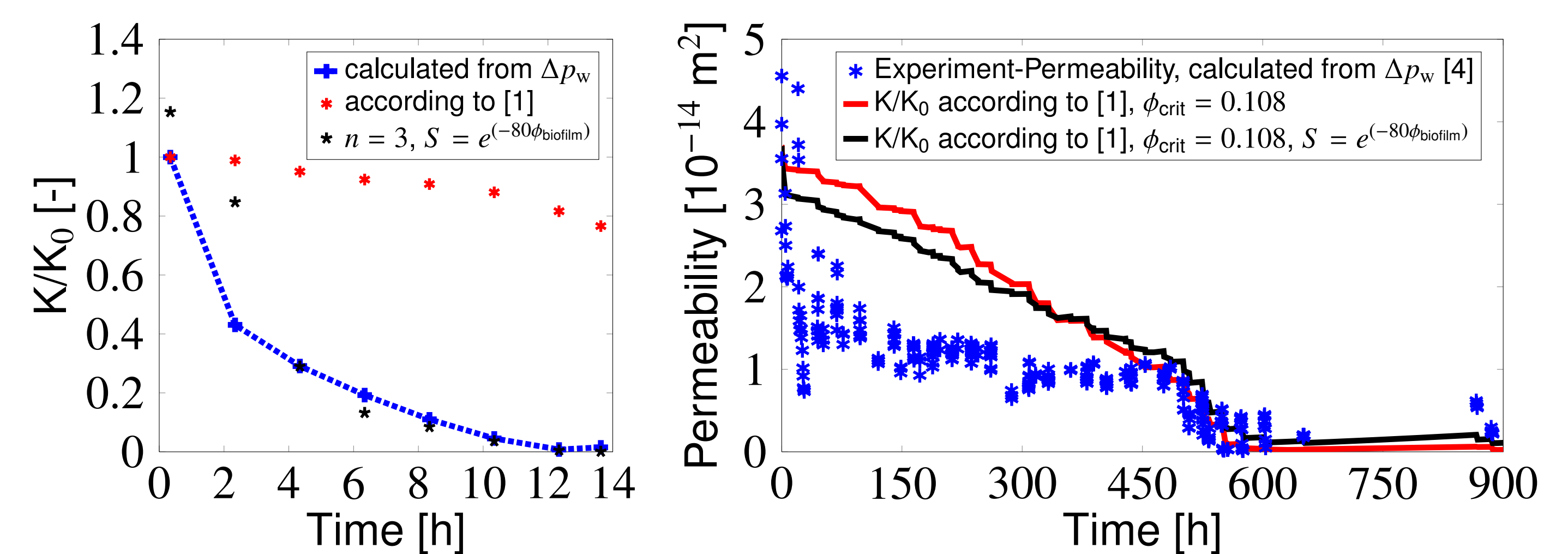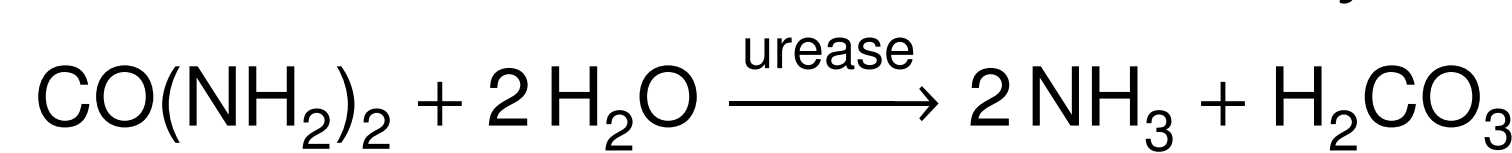
Figure 3: Left: Fit of S to micro flow cell experimental data (collaboration with James Connolly, MSU). Right: Comparison of permeability calculated from measured pressure drop [4] to simulation results with the porosity-permeability relation according to [1] and using S as fitted to the micro flow cell data.

Ureolysis

In recent kinetic studies on the ureolysis by *Sporosarcina pasteurii*,

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

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],

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

the new rate equation according to experiments with whole cells of *S. pasteurii*, as used in MICP applications, is independent of NH_4^+ and H^+ concentrations:

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

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. 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 $c_{a,2}$.
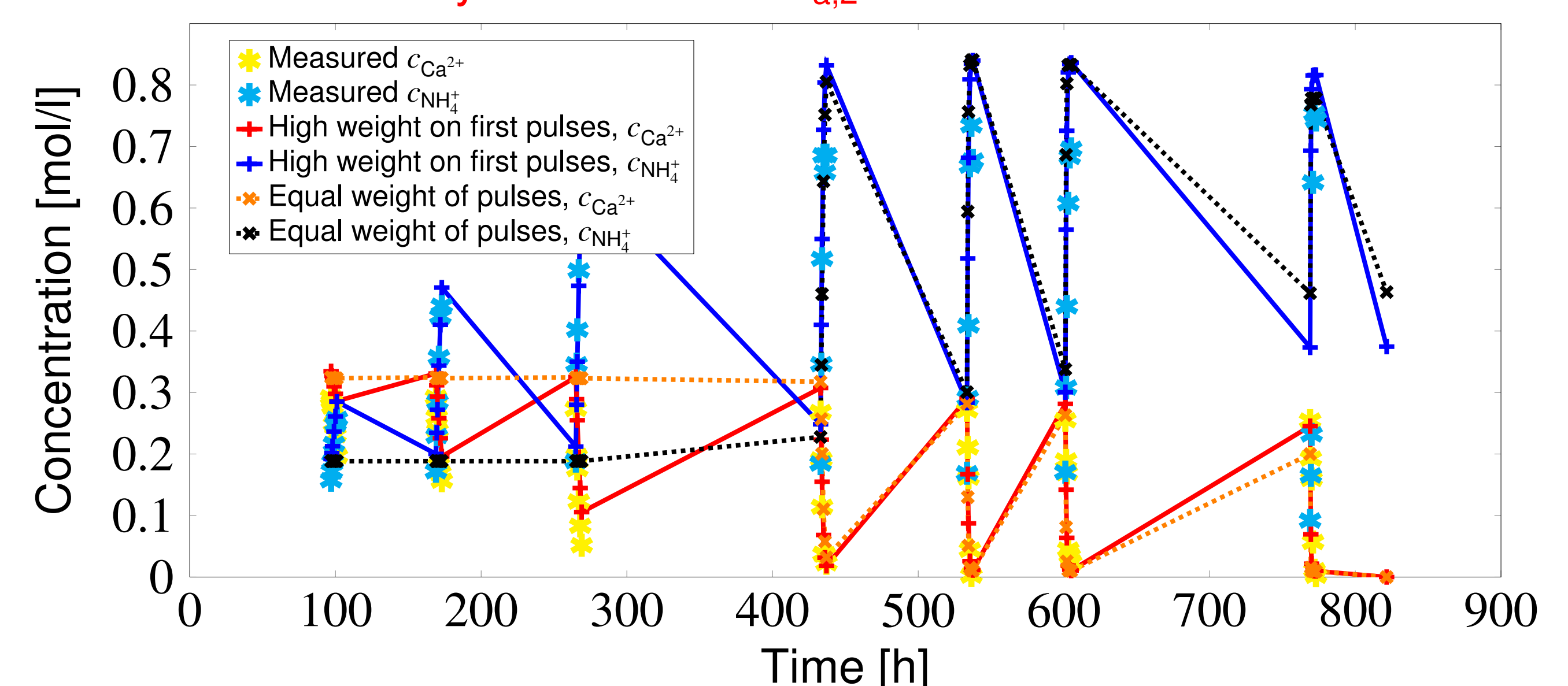
Figure 4: Comparison of measured concentrations at 0.4 m distance from the inlet to two simulation results obtained with different sets of parameters, which were both fitted to experimental data obtained in sand-filled column studies of MICP by Sporosarcina pasteurii conducted at MSU (Ellen Lauchnor).

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.

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[4] Adrienne J. Phillips. *Biofilm-Induced Calcium Carbonate Precipitation: Application in the Subsurface.* PhD thesis, Montana State University, 2013.

[5] 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.