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## Numerical Study Of Microbially Induced Calcite Precipitation As A Leakage Mitigation Solution For CO2 Storage

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### Summary

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In this abstract, we develop simulation models to study and show the potential for field-scale application of microbially induced calcite precipitation (MICP) as a leakage mitigation solution in CO<sub>2</sub> sequestration. Based on laboratory experiments, field-scale cases, and numerical studies from the literature, two injection strategies for efficient MICP are developed: (I) injection of pre-stimulated microorganisms and urea into the subsurface, resulting in calcite precipitation around the body of the microbes; and (II) the classic approach of injecting microorganisms together with chemicals to stimulate growth of biofilm, and subsequent calcite precipitation from the biofilm. To enable field-scale simulations of (I) and (II) at low computational cost, we simplify the processes that have little contribution to the flow, while keeping input parameters and assumptions as realistic as possible. The injection strategies were simulated on field-scale, synthetic 2D radial models. The simulation results showed that both injection strategies produce significant porosity/permeability decrease at targeted locations away from the injection well. Moreover, it was seen that injection strategy (II) produced significantly more porosity/permeability decrease compared to (I).

## Introduction

Storing CO<sub>2</sub> in geological formations has been seen as essential to limit greenhouse gas emissions. To store a large amount of CO<sub>2</sub> over a short period of time using as few injection wells as possible will likely require high injection rates. Consequently, pressure build-ups can reach critical levels, and without pressure relief, near-well fractures or fault reactivation can develop leakage paths in the caprock. Hence, technology to close leakage paths is necessary for safe storage of CO<sub>2</sub>.

A promising sealing technology that has emerged lately is microbially induced calcite precipitation (MICP). In short, MICP creates barriers by converting calcium to calcite (calcium carbonate) from a chemical process catalysed by ureolytic microorganisms and urea. Further barriers can be achieved by growth of biofilms from the microorganisms, if the environmental conditions allow it. The MICP processes have been thoroughly studied on the small scale using laboratory experiments (e.g., Cunningham et al. 2009) and numerical simulations (e.g., Hommel 2016). The technology has also been proven on several field-scale cases, e.g., for groundwater treatment (Fujita et al. 2008), strengthen liquefiable soil (Burbank et al. 2011), sealing of fractures in volcanic rock (Cuthbert et al. 2013) and sandstone reservoir (Phillips et al. 2016).

In this paper, we want to develop numerical simulation models that show the potential of MICP as barrier solution for field-scale CO<sub>2</sub> application. State-of-the-art simulators, like, e.g., Hommel (2016), simulate many of the complex processes involved in MICP with satisfactory match to laboratory experiments. However, replicating field-scale experiments have proven challenging, as well as computationally costly. To enable field-scale simulations, we have identified which microbial systems that are most efficient in reservoir conditions, where there is little (to no) oxygen, high temperature and pressure, etc. The identified microbial systems are converted to mathematical and numerical models, where we have simplified MICP processes with little contribution to the flow, while keeping input parameters and assumptions as realistic as possible. Lastly, the numerical models are run on synthetic test cases where the domains and input parameters are relevant to CO<sub>2</sub> storage problems.

## Microbial systems

On the micro-scale the MICP process is catalysed by ureolytic microorganisms in the presence of urea and calcium. The microbes use the enzyme urease to catalyze the hydrolysis of urea to ammonium and carbonate. The presence of ammonia increases the pH in the microenvironment of the microorganism. This facilitates attachment of calcium ions onto the surface of the cell, due to negative cell charge. Finally, the accumulation of carbonate leads to precipitation of cell-associated calcite (CaCO<sub>3</sub>).

The model organism for MICP is *Sporosarcina pasteurii*, due to its large amount of urease compared to dry cell weight (about 1%), making it a highly effective organism for engineering purposes. Under favourable environmental conditions with access to oxygen, *S. pasteurii* can produce biofilms - a consortium of cells held together by a self-produced matrix. Biofilms act as nucleation sites for the bacteria and gives protection against disinfectants such as CO<sub>2</sub> (Mitchell et al. 2008). In addition to production of calcite within the biofilm, it contributes itself to the clogging of pore spaces. If *S. pasteurii* is injected into an anoxic environment, no - or, at best, limited - biofilm growth can be expected (without injection of substrate and oxygen into the system). Hence, under such conditions, *S. pasteurii* must be cultivated pre-injection for ureolytic activity in the subsurface.

Transport of bacteria in porous systems is a complex process due to the interaction between chemical, mechanical, and hydrological systems. A major challenge is avoiding clogging/cementation of the near-well area. The problem occurs due to uneven distribution of injected bacteria throughout the porous medium. If calcite and (possibly generated) biofilm barriers are established near the injection point, flow to leakage paths beyond the barrier point can be difficult (or even impossible). Many laboratory and numerical experiments have been conducted to study various injection strategies of *S. pasteurii* for MICP, see, e.g., Tobler et al. (2012), Hommel (2016), and Phillips et al. (2016). With the experience

from previous laboratory, field-scale, and numerical experiments in mind, we considered two injection approaches for the field-scale simulations:

- (I) Inject *S. pasteurii* and follow up with injection of urea, with calcite precipitation occurring at the interface between the two.
- (II) Inject *S. pasteurii*, oxygen, and urea with the aim of generating biofilm where the calcite will be produced (assume only calcite precipitation from biofilm)

From an engineering point of view, (I) is simple and cost effective, where the location of calcite precipitation should be easy to control via injection rates and periods. However, repeated injections may be required to achieve complete clogging. Approach (II) is more involved but can ensure a “safer” clogging procedure, since calcite precipitation occurs only in the biofilm. A drawback is the potential for generating biofilm from bacteria native in the reservoir, which can lead to clogging of the injection well. Note that, in both injection approaches, we assume excess calcium and substrate in the system, and model ureolysis rate using the simplified kinetic model in Lauchnor et al. (2015).

## Mathematical and numerical models

Transport of biomass (accumulation of bacteria) and chemicals involved in injection approaches (I) and (II) can be described by

$$\frac{\partial(\phi c^\lambda)}{\partial t} + \nabla \cdot (D \nabla c^\lambda - u c^\lambda) = q^\lambda + Q^\lambda,$$

where  $c^\lambda$  is the concentration,  $D$  is the dispersion tensor,  $u$  is the flux calculated from Darcy’s law (single phase water flow),  $q^\lambda$  is the reaction term,  $Q^\lambda$  is the injection well, and  $\lambda$  indicates a component (biomass or chemical). The clogging process from MICP is described in our system as decrease in porosity and permeability. Reduction in porosity,  $\phi$ , as calcite and/or biofilm,  $\phi_i$ , increases is given by

$$\phi = \phi_0 - \sum_i \phi_i,$$

where  $\phi_0$  is initial porosity. Change in calcite and/or biofilm is given by

$$\frac{\partial \phi_i}{\partial t} = \frac{1}{\rho_i} q^i,$$

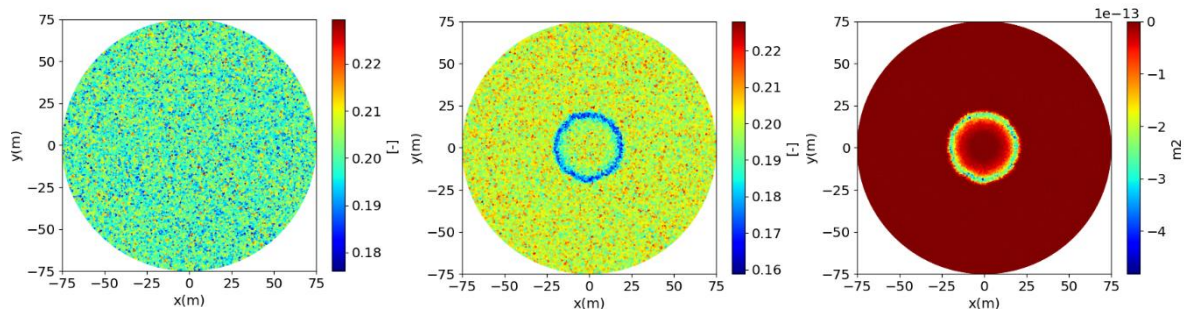
where  $\rho_i$  is the density. Changes in porosity is translated to changes in permeability,  $K$ , through a Konzeny-Carman relation:

$$K = K_0 \left( \frac{\phi - \phi_{crit}}{\phi_0 - \phi_{crit}} \right)^3,$$

where  $K_0$  is initial permeability, and  $\phi_{crit}$  is the critical porosity where the permeability is zero.

In injection approach (I), we only have biomass and urea ( $\lambda = b, u$ ), and calcite ( $i = c$ ), while in (II) we have biomass, urea, and oxygen ( $\lambda = b, u, o$ ), and calcite and biofilm ( $i = c, f$ ). The reaction terms follow the description in Hommel (2016) with the simplifications made at the end of the previous section. The mathematical systems described above are solved numerically with the finite volume solver FiPY.

## Numerical experiments



**Figure 1** Numerical results injection approach (I). Left to right:  $\phi_0$ ,  $\phi$  at the end of simulation, and change in  $K$  from start to end.

We show numerical simulations of field-scale application of injection approaches (I) and (II). The overall goal of the simulations is to show the potential of MICP as a clogging tool for CO<sub>2</sub> leakage. We will not model leakage paths explicitly, but rather show that we can achieve MICP away from the near-well area. The simulations were conducted on a 2D disc domain with lateral spatial directions. Since we are interested in utilizing MICP in the area tens of meters away from the well, the radius of the domain was 75m. The injection well is located at  $(x, y) = (0,0)$  m. The initial porosity ( $\phi_0$ ) and permeability ( $K_0$ ) are heterogeneous and generated from a log-normal distribution. The distributions for  $\phi_0$  lies within the range 0.18-0.22 and within the range  $(0.5-1.5) \times 10^{-12}$  m<sup>2</sup> for  $K_0$ . Furthermore, we set  $\phi_{crit} = 0.1$ . The boundary and initial conditions for all involved components in both injection approaches were set to zero.

In approach (I) we first inject biomass with  $c_{in}^b = 0.01$  mol/m<sup>3</sup> followed up by urea injection with  $c_{in}^u = 5000$  mol/m<sup>3</sup> (with a brief rinse period in between). Both plugs are pushed to the desired location, after which the injection well is shut down. Calcite precipitation will occur at the biomass-urea interface and will be controlled by dispersion in the shut-in period. Total simulation time was 250 h.

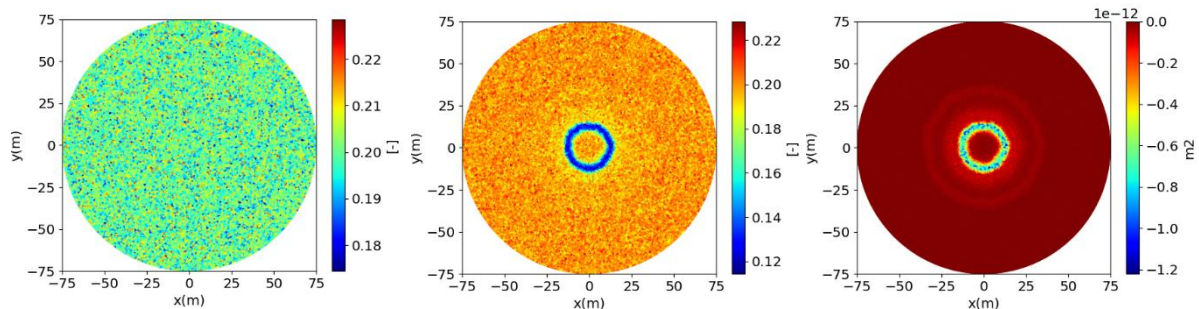
For approach (II) we again start with biomass injection with  $c_{in}^b = 0.01$  mol/m<sup>3</sup>; follow up with oxygen injection with  $c_{in}^o = 0.25$  mol/m<sup>3</sup>; and lastly inject urea with  $c_{in}^u = 5000$  mol/m<sup>3</sup>. In between injecting each component, we have periods of no-flow to grow biofilm (from injection of biomass and oxygen) and produce calcite (from injection of urea). Total simulation time was 400 h.

In Figure 1 the results from injection approach (I) is shown. It is seen that the porosity has decreased considerably. We note that there is no clogging of the well; the porosity decrease happens about 20m from the injection point. The decrease in permeability is also shown, and in some areas it has decrease up to 30 %. Note that, at the end of simulation the MICP processes are very slow (due to slow dispersion rate) but further reduction could be achieved by repeating the injection procedure from the start.

In Figure 2 the results of injection approach (II) is shown. It is seen that the porosity has decreased significantly and occurs away from the injection well as in (I). From the change in permeability we calculated upwards of 80 % reduction in some areas. We note that the decrease in porosity is mostly due to calcite and not biofilm. This is positive since calcite strengthens the rock, compared to pure biofilm barriers.

## Conclusions

In this abstract, we have shown field-scale application of MICP as a clogging tool of leakage paths in CO<sub>2</sub> storage sites. Based on previous studies in the literature on the model bacteria *Sporosarcina pasteurii*, we suggested two injection approaches for efficient MICP: (I) injection of bacteria and urea, with calcite precipitation occurring at the interface of the two; and (II) injection of bacteria, oxygen,



**Figure 2** Numerical results injection approach (II). Left to right:  $\phi_0$ ,  $\phi$  at the end of simulation, and change in  $K$  from start to end.

and urea, with the aim of producing biofilm, and subsequent calcite precipitation from the biofilm. The microbial systems involved in the injection approaches were converted to mathematical and numerical models in a straight-forward manner, ignoring processes with little contribution to the flow situation. Both injection approaches were simulated on a 2D simulation grid using realistic input parameters and assumptions. Simulation results of both injection approaches showed that significant porosity/permeability decrease were generated, away from the injection well, as result of MICP. Comparing injection approach (I) and (II), it is seen that injection approach (II) achieved the most significant porosity/permeability decrease.

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