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Multiphysical numerical modelling of an MICP upscaling experiment with ex-situ hydrolysis

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ABSTRACT

Microbially induced calcite precipitation (MICP) is an innovative biogeochemical ground improvement technology that can be used in-situ to improve soil stiffness and strength, by precipitating calcite within the soil. Bio-chemo-hydro-mechanical processes are key aspects of this technology, which makes the use of advanced numerical models necessary to optimize the treatment design. In this study, an upscaling experiment was modelled using a multiphysical framework. The upscaling experiment used a novel treatment strategy, based on ex-situ hydrolysis, which required a novel bio-chemical reactive transport formulation. Numerical evaluations in both 2D and 3D were used to properly account for the geometry and injection strategy of the experiment. Modelling results were compared with the experimentally measured properties. Both models showed that the injection pressures during the consecutive injections of 20 m^3 of reactive batches could well be replicated. Modelling in 3D increased the understanding of the influence of the applied treatment strategy on the overall precipitation pattern. Overall, the numerical model was capable of capturing the evolution of the precipitation process as a response to the variation of chemical, hydraulic and mechanical conditions, which validates the use of the numerical framework as an effective strategy for understanding, predicting and optimizing the MICP treatment with ex-situ hydrolysis.

Keywords: Multiphysics, MICP, Numerical modelling

1 INTRODUCTION

Ground improvement is an important topic in geotechnical engineering for meeting the demands of construction industry. It allows to build on sites where this was previously not possible. Moreover, it can help stabilize slopes and prevent erosion. An environmentally friendly alternative to cement injection as an improvement method is using microbially induced calcite precipitation (MICP), which has been a growing research topic in recent years. This novel in-situ technology relies on two reactions, hydrolysis of urea, (1) and precipitation of calcium carbonate, (2):

$$CO(NH_2)_2 + 2H_2O \xrightarrow{\text{urease}} CO_3^{2-} + 2NH_4^+ \tag{1}$$

$$CO_3^{2-} + Ca^{2+} \rightarrow CaCO_3 \downarrow \tag{2}$$

Calcite produced through this process can precipitate at the surface of soil grains, covering particle surfaces and can form bonds between adjoining grains at their contact points. It is well established that the precipitation of calcite through MICP creates a cemented, more densified soil with improved mechanical properties, like its stiffness and strength (e.g., Cui et al. 2017, Mortensen and DeJong 2011).

One of the main challenges for the large-scale application of MICP is possibly having undesired by-products in the groundwater, mainly residual ammonium concentrations resulting from the urea hydrolysis reaction (DeJong et al. 2010; DeJong et al. 2014). To tackle this aspect, Terzis and Laloui (2021) proposed a new strategy for the deployment of MICP, relying on ex-situ hydrolysis. This novel strategy was applied in an upscaling experiment reported in Harran et al. (under review). With this procedure, urea hydrolysis occurs ex-situ in a bioreactor instead of in the soil. This enables the control of the biowaste stream, offering the opportunity for proper extraction of ammonium and better monitoring of the hydrolysis reaction.

Numerical modelling of this innovative soil-strengthening technology serves two important purposes. First, it allows testing of the theoretical models proposed for MICP. Secondly, advanced numerical modelling can be valuable as a predictive tool for optimizing treatment strategies. Full-scale experiments are difficult and often costly to perform, whereas through numerical simulations, many different boundary and initial conditions can easily be explored to design optimal treatment with MICP.

Efforts of many authors have resulted in the development of several modelling frameworks representing relevant chemical, biological, hydrological and mechanical phenomena occurring during the MICP treatment. In particular, numerical modelling of MICP at field scale, including a comparison of the model results with experimental data to verify the proposed modelling methodology, has been performed in several studies (Van Wijngaarden et al. 2016; Minto et al. 2019; Zeng et al. 2021). Many of these models have been developed with varying objectives.

In the aforementioned numerical studies, the two reactions (1) and (2) were implemented in a simplified manner by using one overall net reaction equation with one reaction rate. This modelling strategy cannot be applied to the upscaling experiment from Harran et al. (under review), since the novel ex-situ treatment scheme was used. This means that only equation (2) is a relevant in-situ process that should be accounted for. The present study, therefore, presents a numerical framework targeted to simulate MICP treatment with ex-situ hydrolysis to evaluate this upscaling experiment and cannot be compared with other previously presented frameworks that use one net reaction equation. The study objective is to demonstrate that numerical modelling is an effective tool for predicting the MICP process with ex-situ hydrolysis for future applications.

2 METHODOLOGY

2.1 Theoretical framework

A multiphysical modelling framework is used to simulate the ex-situ MICP treatment. The chemical components are introduced into the soil through injections of solutions, after which the chemical reactions led to calcite precipitation. For this reason, transport of the fluid, transport of the diluted species within the fluid, and chemistry are evaluated in the model. The modelling framework includes mass balances for the fluid, (3) and for each of the species, (5)

$$\frac{\partial \phi \rho}{\partial t} + \nabla(\rho \boldsymbol{u}) = 0 \tag{3}$$

where ϕ is the porosity (-) and ρ is the fluid density (kg/m^3). Here **u** is the specific discharge of the fluid (m/s), which can be described by Darcy's law including gravity effects, (4)

$$u = -\frac{k_{hydr}\mathrm{I}}{\rho g}(\nabla p + \rho g) \tag{4}$$

in which k_{hydr} is the hydraulic conductivity in the porous medium (m/s), p is the fluid pressure (Pa) and g is the gravity vector (m/s^2). The mass balance for the diluted species in the liquid, carbonate, calcium and calcium carbonate, is given in (5) and includes advection, diffusion and dispersion:

$$\frac{\partial \phi c_i}{\partial t} + \boldsymbol{u} \cdot \nabla c_i = \nabla \cdot \left(\mathrm{I} D_{e,i} \nabla c_i\right) + r_i + S_i \tag{5}$$

where c_i and r_i are the concentration of species i (mol/m^3) and its reaction rate (mol/(m^3·s)) respectively and S_i is a source term (mol/m^3/s). $D_{e,i}$ is the effective diffusivity (m^2/s) which is calculated using (6)

$$D_{e,i} = \frac{\phi}{\tau} D_{c,i} \tag{6}$$

with τ the tortuosity of the porous media and $D_{c,i}$ the diffusivity coefficient of species i, which is deducted from the chemical properties of the species. The tortuosity is defined based on the Millington and Quick model (Millington and Quirk, 1961), (7).

$$\tau = \phi^{-1/3} \tag{7}$$

For the purposes of this work, the biological aspect does not need to be accounted for, as it is not relevant for an application with ex-situ hydrolysis. Chemical considerations are accounted for through the reaction rate for the precipitation reaction which can be computed using (8), similar to Nassar et al. (2018):

$$r_p = k_p(\Omega - 1) \text{ with } \Omega = \frac{c_{ca^{2+}} + c_{CO_3^{2-}}}{K_{sp}} \tag{8}$$

where k_p is the precipitation kinetic constant (mol/m^3/s) and K_{sp} is the calcite solubility constant with a value of $10^{-8.48}$ mol^2/m^6 (e.g, Nasser et al. 2018). A value of 5.8E-9 mol/m^3/s was used in this study for the precipitation kinetic constant. The porosity in the model is a function of the amount of produced calcite through the following relation, (9), as in Fauriel and Laloui (2013), Van Wijngaarden et al. (2016) and Wang and Nackenhorst (2020)

$$\frac{\partial \phi}{\partial t} = -\phi r_p \frac{M_{CaCO_3}}{\rho_{CaCO_3}} \tag{9}$$

with M_{CaCO_3} being the molar mass of calcite (kg/mol) and ρ_{CaCO_3} the calcite density (kg/m^3). The reduction in porosity resulting from the precipitation of calcium carbonate affects the hydraulic conductivity of the porous medium. In this model, the evolution of the hydraulic conductivity is described based on the Kozeny-Carman relationship with (10)

$$k_{hyd} = k_{hyd,0} \frac{\phi^3}{(1-\phi)^2} \frac{(1-\phi_0)^2}{\phi_0^3} \tag{10}$$

where $k_{hyd,0}$ is the initial hydraulic conductivity (m/s) and ϕ_0 is the initial porosity (-).

2.2 Numerical model of the in-situ upscaling experiment

A large-scale experiment to address upscaling challenges of MICP was performed by Harran et al. (under review). They applied an ex-situ hydrolysis injection strategy, in which carbonate species were injected rather than bacteria and urea. A 60 m^3 saturated sand domain with a density of 1560 kg/m^3 was treated through injections with 20.8 m^3 of treatment solutions, which is approximately one pore volume of the sand body. The solutions were injected at eight injection locations at three different depths, through a three-dimensional injection pattern. The effluent was extracted by gravity through drains at the bottom of the setup. The sand used in the experiment was labelled poorly graded according to ASTM D2487.

Two finite-element models, a 2D model and a 3D model, are used in this study to simulate the upscaling experiment. Both models are developed in COMSOL Multiphysics 6.0 (COMSOL, 2020). 3D evaluation of the experiment was included to evaluate the precision of the 2D analysis, that is unable to represent the exact injection strategy. The features of both models are presented in the following sections.

2.2.1 2D model

A representative section with injection and extraction points was evaluated in the 2D analysis. The model dimensions, initial and boundary conditions are shown in Figure 1. The porosity and hydraulic conductivity were both assumed as initially homogeneous over the porous medium. The mesh used for the simulations was composed of 35016 domain elements, and 616 edge and vertex elements.

One injection cycle in the model considers the injection of the calcium solution with a concentration of 1.1M in one tube (with three vertically aligned injection points) while injecting the carbonate solution with the same concentration of 1.1M in the other tube. These injections are done with an inflow of 5 L/min for each tube. The solutions were then alternated in the next injection cycle. In total 12 injection cycles were simulated in this 2D model, which is representative for most injection wells in the performed experiment from Harran et al. (under review).

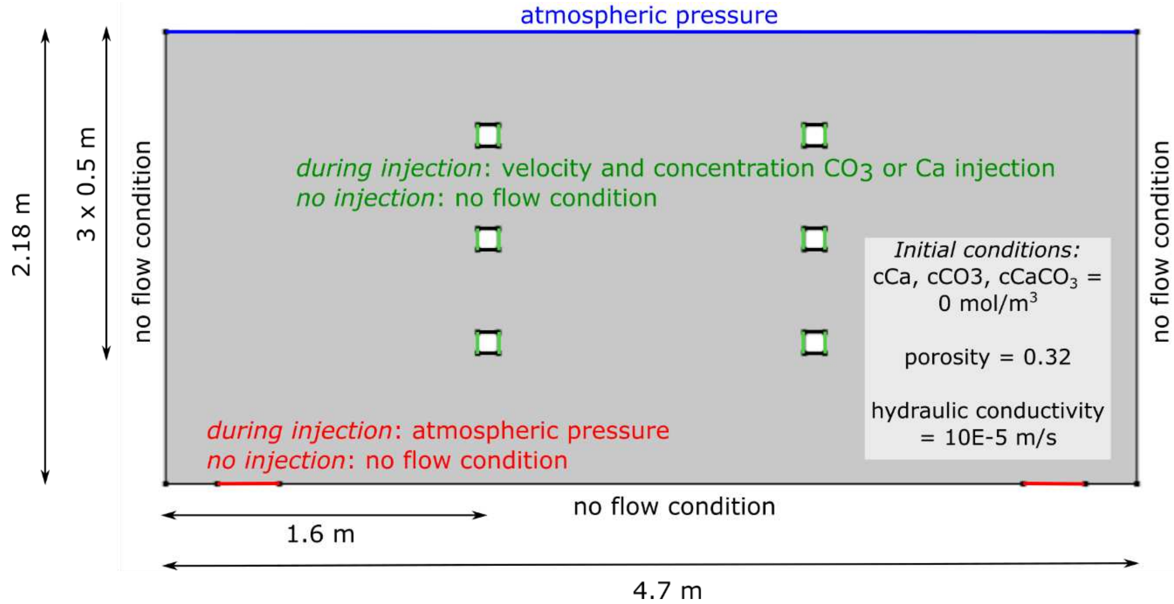

Figure 1. *2D numerical model setup including applied boundary and initial conditions*

2.2.2 3D model

The full experimental setup was also evaluated using a 3D model to properly account for the geometry of the experiment. Figure 2 shows the model dimensions and boundary conditions used in this simulation. The initial conditions were the same as those used in the abovementioned 2D simulation. The mesh was composed of 1357008 domain elements and 4114 edge and vertex elements.

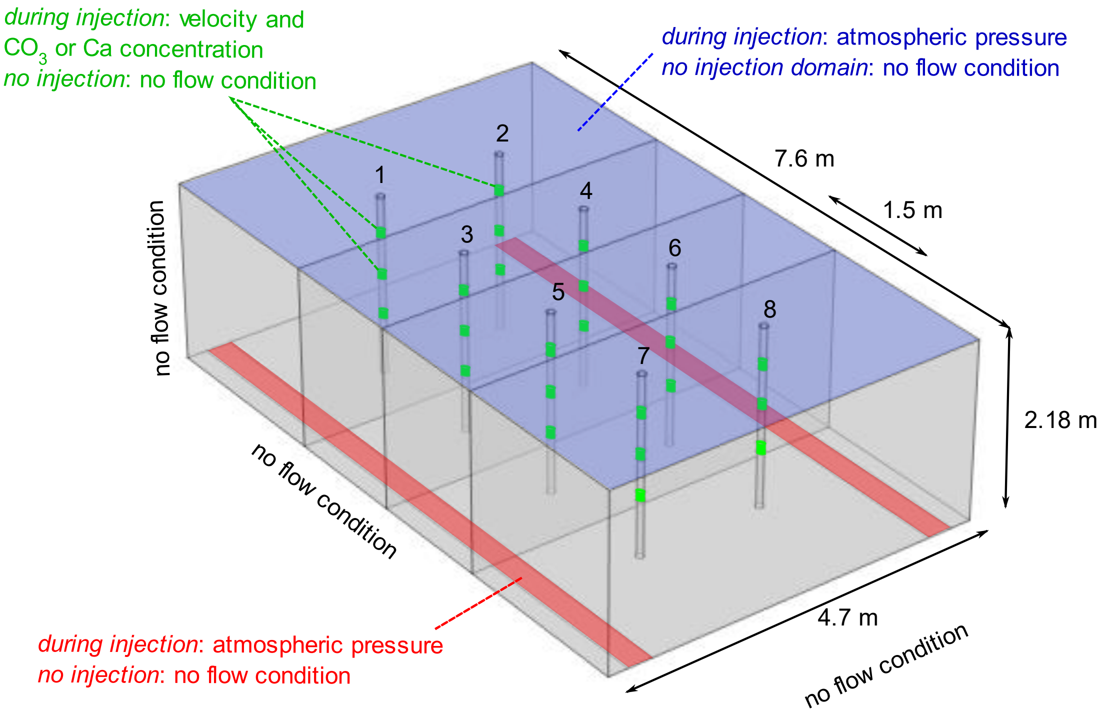

Figure 2. *3D numerical model setup including applied boundary and initial conditions*

The injection pattern for the 3D analysis consisted of several consecutive injections for each injection well, numbered in Figure 2. On a typical injection day, two injections (one with calcium solution and one with carbonate solution) were done in four wells. Table 1 provides an overview of the injection pattern implemented in the 3D model, according to the performed upscaling experiment.

Table 1. *Injection pattern of the upscaling experiment of Harran et al. (under review) that was implemented in the 3D model*

	Injection day														Total injections
Injection wells	1	2	3	4	5	6	7	8	9	10	11	12	13	14	
1, 2	X	X			X	X			X	X			X	X	16
3, 4		X	X			X	X			X	X				12
5, 6			X	X			X	X			X	X			12
7, 8				X	X			X	X			X	X		12

3 MODELLING RESULTS

Harran et al. (under review) measured the injection pressures during the injection cycles of the treatment solutions. These experimentally obtained injection pressures were compared to the pressures obtained from the 2D and 3D numerical simulations, as presented in Figure 3.

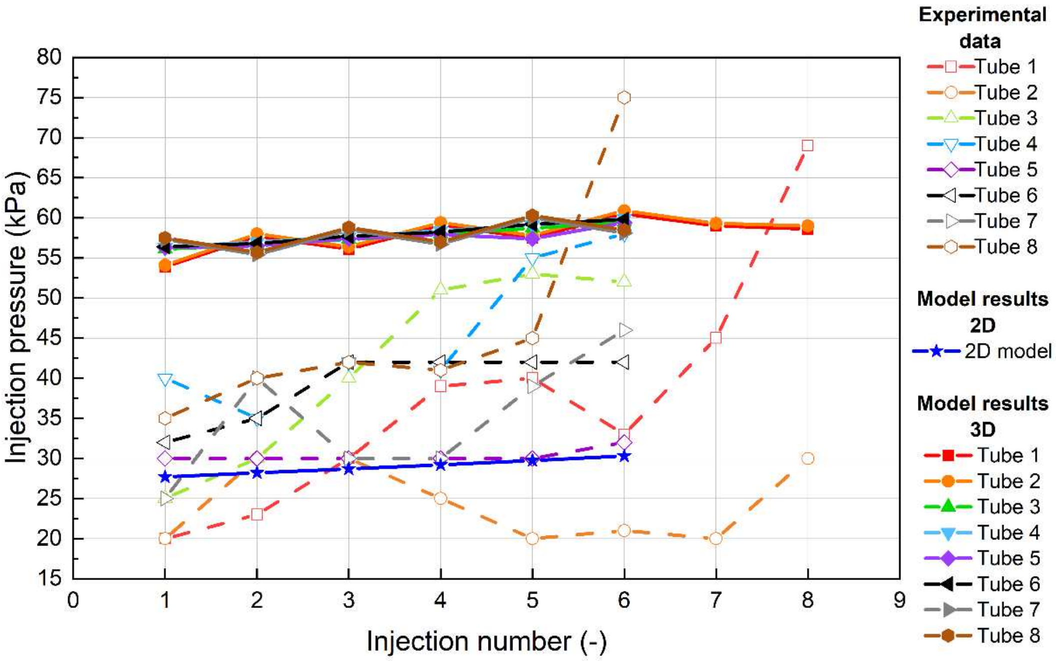

Figure 3. *Comparison of injection pressures over time as measured by Harran et al. (under review) with 2D and 3D model results*

The 2D model captured the right range of the injection pressure over time. A small increase in pressure over time is obtained in the model, due to the calcite precipitation which caused a reduction in hydraulic conductivity. The experimental results showed more variation of the injection pressures over time due to also local behaviour, an example is soil erosion around injection points that occurred in the experiment. The pressures obtained with the 3D simulations are higher than the injection pressures obtained with the 2D model simulations and most experimentally observed values, but they are still within the range of measurements. An important aspect here is the interaction effects between injection points that are not considered in the 2D simulation, but could be evaluated for the 3D study.

In the work of Harran et al. (under review) the change in penetration resistance between the treated and untreated soil domain caused by the precipitation of calcite was evaluated at different locations to evaluate the MICP treatment. These experimental results of penetration resistance were qualitatively compared with calcite precipitation patterns obtained in this study. Figure 4 and 5 show the calcite content distributions obtained with the 2D and 3D numerical models in a similar cross-section. Figure 6 and 7 show the precipitation pattern for the other model dimensions of the three-dimensional analysis.

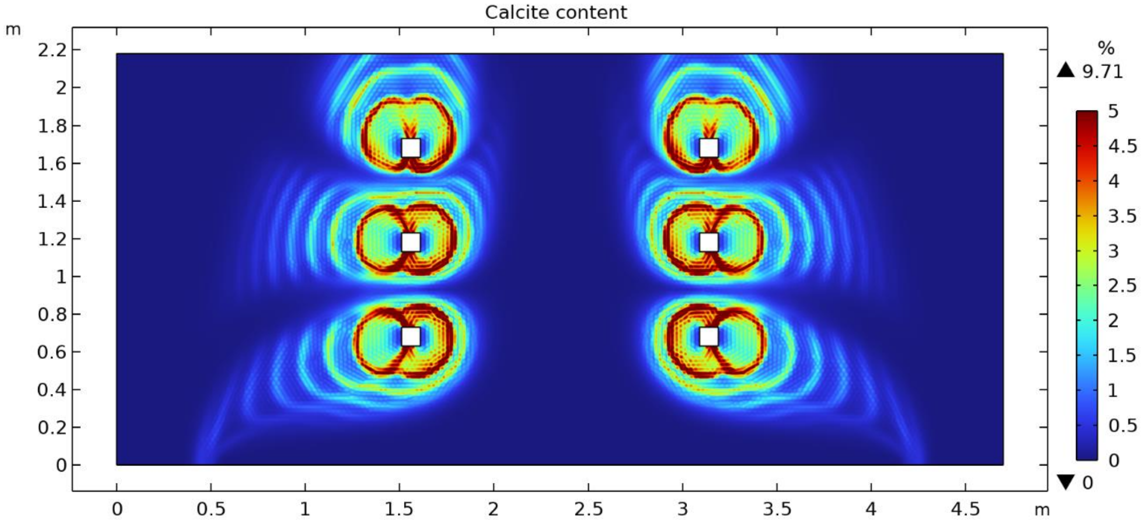

Figure 4. *Calcite content obtained through the two-dimensional simulation*

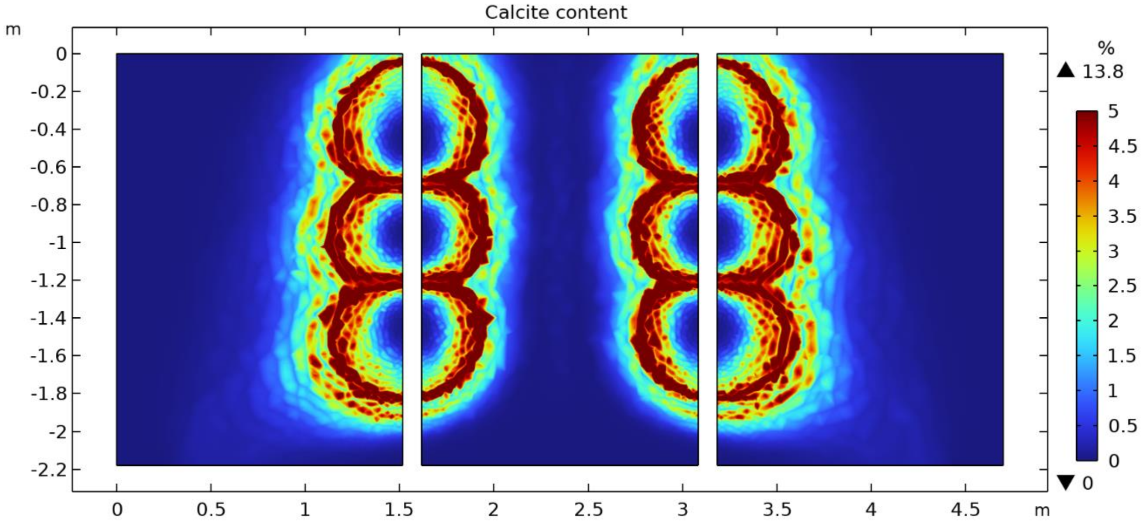

Figure 5. *Calcite content obtained through the three-dimensional simulations, in the cross section with injection points 5 (left) and 6 (right)*

Comparing the 2D and 3D simulations shows some differences, looking at a slice of the 3D model that is representative of the 2D model geometry (Figure 5). In the three-dimensional simulation, flow also occurred in this section when there was an injection in any other zone of the soil domain. This has an influence on the precipitation pattern in the simulation as a consequence of the interaction between injection wells in different planes, highlighting the need for a three-dimensional evaluation of this injection strategy.

The higher number of total injections in injection wells 1 and 2 compared to the other injection points is reflected in the calcite content obtained with the 3D simulation, as shown in Figure 6 and 7. Injection wells 1 and 2 have a slightly larger area with a calcite percentage of at least 5% around the injection well.

Harran et al. (under review) reported the most notable enhancements of the tip resistance close to the injection wells and lower enhancements along the centreline due to the drainage conditions. This pattern is well captured by both the 2D and 3D model. Along the centreline of the basin, no calcite precipitated for both models, and a zone with higher calcite precipitation is found around the injection points. Other zones with notable enhancement of penetration resistance mentioned were towards the drains with higher overburden and near the surface of the basin due to percolation and ponding effects. The first is well replicated in both the two- and three-dimensional evaluations, with a higher calcite content towards the outlets of the model. Higher precipitation at the top surface of the basin resulted from ponding effects.

This was not captured by the model as the soil-atmosphere interactions were simplified to constant water pressure, resulting in a net outflow from the top.

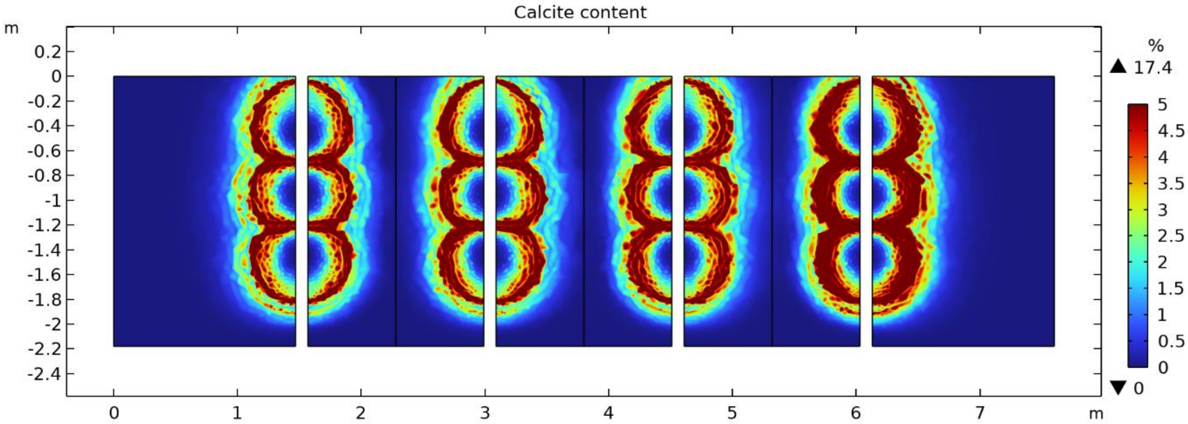

Figure 6. *Calcite content obtained through three-dimensional simulations, in a longitudinal cross-section with injection points 1 (right), 3, 5 and 7 (left)*

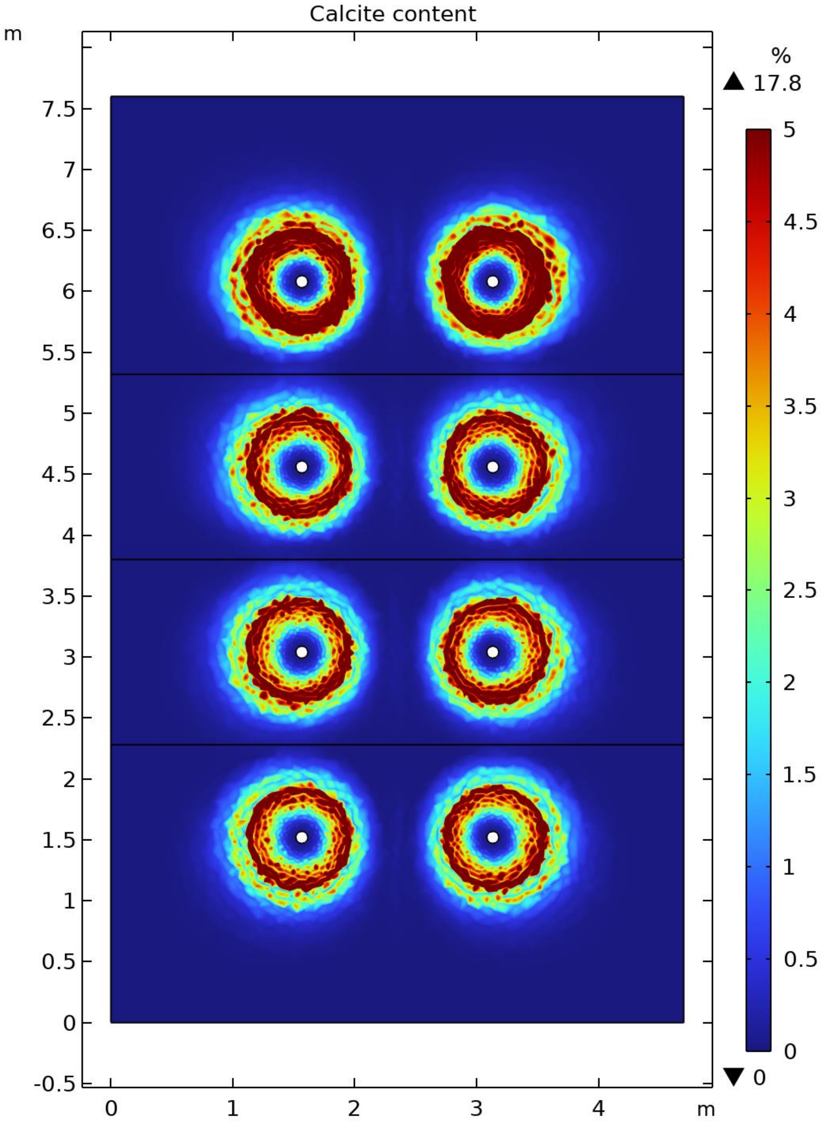

Figure 6. *Calcite content obtained through three-dimensional simulations, a planar slice of the basin showing all injection points from 1 (left top) to 8 (right bottom)*

4 CONCLUSIONS

This study focused on the challenge of modelling biocementation and proposed a modelling framework to evaluate projects with an ex-situ hydrolysis treatment scheme. The framework was used to model an upscaling experiment consisting of the treatment of a 60 m^3 sand domain. Results from both the 2D and 3D model simulations were compared with the experimentally obtained results. Both the two-dimensional and three-dimensional studies could well replicate the injection pressures and precipitation pattern of the experiment. By including the third dimension in the study, interaction effects between injection points during different injections were identified and the injection pattern was better replicated. The main finding of this study is that the applied numerical framework is capable of capturing the evolution of the precipitation process as a response to the injections in the basin. The numerical framework is validated as an effective strategy for understanding and predicting the MICP process with ex-situ hydrolysis.

5 ACKNOWLEDGEMENTS

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REFERENCES

COMSOL (2020). COMSOL Multiphysics® version 6.0: User's guide and reference manual. Burlington, Massachusetts, United States: COMSOL

Cui, M. J., Zheng, J. J., Zhang, R. J., Lai, H. J., & Zhang, J. (2017). Influence of cementation level on the strength behaviour of bio-cemented sand. *Acta Geotechnica*, 12, 971-986.

DeJong, J. T., Mortensen, B. M., Martinez, B. C., & Nelson, D. C. (2010). Bio-mediated soil improvement. *Ecological Engineering*, 36(2), 197-210.

DeJong, J. T., Soga, K., Kavazanjian, E., Burns, S., Van Paassen, L. A., Al Qabany, A., ... & Weaver, T. (2014). Biogeochemical processes and geotechnical applications: progress, opportunities and challenges. In *Bio-and chemo-mechanical processes in geotechnical engineering: géotechnique symposium in print 2013* (pp. 143-157). Ice Publishing.

Fauriel, S., & Laloui, L. (2012). A bio-chemo-hydro-mechanical model for microbially induced calcite precipitation in soils. *Computers and Geotechnics, 46, 104-120.*

Harran, R., Terzis, D., Laloui, L. (under review). Addressing the Challenges of Homogeneity, Quality Control, and Waste Elimination in Soil Bio-improvement: A Large-scale Experiment.

Millington, R. J., & Quirk, J. P. (1961). Permeability of porous solids. *Transactions of the Faraday Society, 57, 1200-1207.*

Minto, J. M., Lunn, R. J., & El Mountassir, G. (2019). Development of a reactive transport model for field-scale simulation of microbially induced carbonate precipitation. *Water Resources Research*, *55*(8), 7229-7245.

Mortensen, B. M., & DeJong, J. T. (2011). Strength and stiffness of MICP treated sand subjected to various stress paths. In Geo-Frontiers 2011: *Advances in geotechnical engineering* (pp. 4012-4020).

Nassar, M. K., Gurung, D., Bastani, M., Ginn, T. R., Shafei, B., Gomez, M. G., ... & DeJong, J. T. (2018). Large-scale experiments in microbially induced calcite precipitation (MICP): Reactive transport model development and prediction. *Water Resources Research*, *54*(1), 480-500.

Terzis, D. and Laloui, L. (2021). *Method and system for producing a carbonate-containing species-rich, nitrogen-containing species-free solution* (Patent No. WO2021234434).

Van Wijngaarden, W. K., Van Paassen, L. A., Vermolen, F. J., Van Meurs, G. A. M., & Vuik, C. (2016). A reactive transport model for biogrout compared to experimental data. *Transport in Porous Media*, *111*(3), 627-648.

Wang, X., & Nackenhorst, U. (2020). A coupled bio-chemo-hydraulic model to predict porosity and permeability reduction during microbially induced calcite precipitation. *Advances in Water Resources*, *140*, 103563.

Zeng C. et al (2021). Experimental and numerical analysis of a field trial application of microbially induced calcite precipitation for ground stabilization. *J. Geotech. Geoenviron. Eng, 147(7)*: 05021003.

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