NUMERICAL MODELLING OF BIOCEMENTATION UPSCALING EXPERIMENT: INSIGHTS FROM VARIED INJECTION STRATEGIES

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KEYWORDS

Numerical modelling, biocementation, field-scale, multiphysics

ABSTRACT

Biocementation through microbially induced calcite precipitation (MICP) is an innovative technology using the precipitation of calcium carbonate, leading to improved soil strength and stiffness. A recently performed upscaling experiment aimed to evaluate the efficacy of diverse injection methods for enhancing the calcite content distribution within an initially unsaturated soil domain. This study evaluates the experiment using numerical modelling, to better understand the complex processes involved and interpret the influence of injection variations. The multiphysical framework represents the bio-hydro-chemical processes of MICP and their couplings. An extensive monitoring campaign allows for a multilevel validation of the modelling approach. Modelling results show that the hydraulic aspect of the injections in the initially unsaturated soil domain could be replicated. The distribution of calcite content and DPT results corroborate the zone of improvement observed in the numerical and experimental data. Additionally, numerical modelling helps to unravel the multiphysical processes in this large-scale field experiment allowing for interpretation of variations in reaction rates and bacteria distribution arising from diverse injection strategies. In this aspect, this study contributes to the development of a numerical framework to serve field-scale, geotechnical applications and contribute to the critical aspects of treatment design and optimization as well as quality assessment and control.

1. INTRODUCTION

Biocementation for ground improvement is a rapidly advancing area of research, offering an environmentally friendly solution surpassing conventional

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ground improvement methods' limitations. Utilising ureolysis-based MICP targets the formation of calcium carbonate in the soil through two key reactions. Urea hydrolysis (eq.1), catalysed by the enzyme urease, increases pH and forms carbonate and ammonium ions, followed by calcium carbonate precipitation (eq.2) in a calcium-supersaturated environment.

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

$$CO_3^{2-} + Ca^{2+} \rightarrow CaCO_3 (s)$$
⁽²⁾

Calcite, the most stable polymorph of calcium carbonate under typical conditions [1], forms within the soil matrix, enhancing soil density and forming bonds between particles. This technology finds applications in the fields of soil strengthening, slope stabilization, liquefaction control and erosion control amongst others.

Designing MICP treatments poses challenges due to complex biochemical processes, necessitating sophisticated tools. Many researchers have developed modelling frameworks encompassing chemical, biological, hydrological, and mechanical processes and their interactions (e.g. [2 - 4]). However, studies often rely on 2D simulations validated with lab-scale samples, which may not accurately capture the complexities in large-scale MICP applications.

Only recently some works began to explore design choices in injection timings and bacteria concentrations using modelling frameworks [5,6], but a comprehensive investigation of the influence of all design parameters on the treatment outcomes remains to be understood. To address this aspect, this work presents a modelling campaign replicating an upscaling experiment described in Büyüklü et al. (2023) [7] where variations in injection rate, volume of injected solutions and injection methods were used.

2. METHODOLOGY

Theoretical framework

A multiphysical framework including hydraulic, chemical and biological components is used, an overview is presented in Figure 1. Modelling is done with COMSOL Multiphysics vs. 6.2 [8].

The upscaling experiment, initially under unsaturated conditions, necessitates the use of Richards' equation. The Van Genuchten model is used to describe soil water retention and its influence on hydraulic conductivity, akin to Faeli et al. (2023) [9]. Initial Van Genuchten model parameters derive from the grain size distribution of the porous material, with final adjustments made based on calibration with pore water pressure measurements while ensuring realistic values. Mass conservation equations address the transport of diluted species, accounting for diffusion, dispersion, and convection within the variably saturated



Figure 1, Overview of multiphysical modelling framework.

domain. Initially suspended in the injected solution, bacteria distribution is then governed by attachment, decay, and transport. Variations in concentrations over time are modelled using attachment and decay rates, assumed constant as per existing literature (e.g., [5,10]). The urea hydrolysis rate follows Michaelis-Menten kinetics, dependent on bacteria and urea concentrations, and the precipitation rate is defined using carbonate and calcium concentrations. A reduction factor, calibrated from various studies [11,12], is used in the precipitation rate to account for chemical and biological simplifications. A coupling includes the reduction in porosity and saturated hydraulic conductivity as result of calcite precipitation, the latter described using a Kozeny-Carman relationship. Model parameters are based on literature values and not calibrated apart from the ones indicated in this section.

Model of the upscaling experiment

Büyüklü et al. (2023) [7] explored the impact of different MICP solution injection settings and techniques on calcite precipitation distributions. Several injection wells, each varying in flow rates, design, the number of injections or the volume of the injected solutions, were employed. A comprehensive monitoring campaign included the use of piezometers, dynamic penetrometer resistance (DPT) measurements and soil sampling for measurements of calcite content around one of the wells.

The injection wells are modelled as individual experiments using a 2D axisymmetric approach, facilitated by the absence of interactions between wells or walls of the setup. Figure 2 illustrates the general setup of the models, and depicts varied injection configurations and piezometer placements to replicate



Figure 2, 2D axisymmetric general model geometry and variations to include different injection techniques and piezometer locations.

specific experimental settings for each well. Time-dependent boundary conditions at inflow points mimic the injection patterns applied, specifying relevant flow rates and concentrations of the solutions.

Each model employs a different mesh to accommodate slight geometry variations, but similar mesh quality is ensured. Simulations span from the first injection to the moment of quantification of soil improvement, i.e., the time when DPT testing was performed.

3. RESULTS

The extensive monitoring campaign allows a detailed comparison between experimental and numerical results.

Pore water pressure profiles obtained with the piezometers are compared with numerically obtained profiles at the representative locations. Results for the piezometers located in proximity to well 2 are presented in Figure 3. For all wells, the profile of improvement obtained through the model can be compared with experimental improvement ranges obtained from the DPT measurements and observations. Numerically obtained calcite profiles for the wells are presented in Figure 4 and an image capturing the experimentally obtained soil columns is presented in Figure 5. Moving to a quantitative analysis, a comparison in terms of calcite content profile surrounding one of the wells was possible after examining the calcite contents of 21 soil samples at varying heights and radii from



Figure 3, Comparison of experimental and numerically obtained pore water pressures at varying locations in proximity to well 2, at locations as shown in Figure 2.

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well 3 using gravimetric acid digestion. A comparison between these experimental and numerical results is presented in Figure 6.



Figure 4, Model predictions of calcite content profiles as result of the treatments applied.



Figure 5, Sand columns obtained as a result of the MICP treatment applied in the upscaling experiment of Büyüklü et al. (2023) [7].

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Figure 6, Calcite content for sampling points obtained with (left) experimental campaign and (right) the modelling result.

4. **DISCUSSION**

The comparison of pore pressure profiles in Figure 3 shows negative pore pressures relative to atmospheric pressure due to the unsaturated conditions. For locations higher in the soil profile the model initially predicts larger negative pressures, compared to the experimental observations. This is likely due to the starting point of the model not capturing potential influences of rainfall and an initial degree of saturation of the soil before the start of the injections in the experiment. Despite this initial difference, it can be seen that the framework can sufficiently capture the changes in pore water pressures across the soil domain as a result of the MICP treatment by means of injections of solutions.

Figure 6 shows a trend in the experimental measurements of increasing calcite content for deeper positions within the soil profile. This trend is also captured by the model; however, there is a lower variability in the predicted calcite contents compared to the experimental values. Potential sources of error stem primarily from experimental procedures, as gravimetric acid digestion was applied to a soil with a significant natural carbonate content in the untreated state and a relatively high content of fines.

DPT measurements and visual inspection of the soil columns (Figure 5) revealed smaller soil improvement radii for well 1 and 2 compared to wells 3, 4 and 5, along with higher tip resistances around well 3 [7]. Additionally, injecting larger solution volumes, as applied in well 2, did not notably impact soil improvement in terms of radius and resistance. The treatment applied to well 4, using the novel injection technique with a slitted pipe, resulted in a more homogeneous precipitation pattern over the height.

The bio-chemo-hydro framework replicates these qualitative observations (Figure 4), with higher calcite contents and larger improvement radii around well 3. This is primarily attributed to the utilization of a higher injection rate and the use of multiple cycles of cementation solution injection. The model provides further insights, explaining why for instance increased solution volumes in well 2 had minimal effect: low injection rates during bacterial solution injection resulted in a smaller radius of bacterial attachment, while higher flow rates were used during cementation solution injection. Modelling highlights the complex interplay between the injection rate used and bacteria attachment, which then governs the spatial variation of the urea hydrolysis reaction rate. Similar to the experiment, lower calcite contents are obtained for wells 4 and 5, but the distribution is noted at a larger radial distance from the well and is more homogeneous over depth.

Nonetheless, some disparities persist between experimental and numerical findings, notably in some cases the distance of improvement from the well is overestimated by the model compared to the expected distance based on the DPT campaign. It is expected that these discrepancies partly stem from observed behaviour that cannot be replicated, such as surface settlement upon fluid injections, erosion of soil near injection points, and non-functioning injection outlets, which were all observed in the upscaling experiment.

5. CONCLUSIONS

This study aims to demonstrate the capabilities of a modelling framework to capture key trends observed in a large-scale experiment and to enhance understanding of variables to ultimately master the design of MICP treatment. Main trends in pore water pressures, and calcite content distributions are captured, while highlighting the key role of the used injection rate. Thereby, this study aids in advancing modelling tailored for field-scale MICP applications.

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