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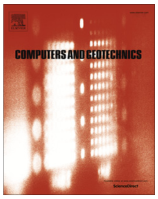

Bio-geochemical reactive transport modeling of microbial induced calcite precipitation to predict the treatment of sand in one-dimensional flow

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ABSTRACT

Microbial induced calcite precipitation (MICP) has been well studied to date in the laboratory as a viable alternative soil improvement technique that harnesses a natural bacterial process to induce cementation. Specifically, MICP utilizes the microbial process of hydrolysis of urea to induce pH increase leading to calcite precipitation. The study presented herein demonstrates the utility of a simple bio-geochemical reactive transport model to predict MICP in one-dimensional column experiments. The mathematical model was originally developed in the framework of the TOUGHREACT code to include kinetically controlled reaction rates for urea hydrolysis and calcite precipitation. Inverse modeling, via UCODE-2005, is utilized to calibrate and verify the model to experimental data including aqueous and mineral chemistry. Results indicate good agreement between data and simulated results for capturing the trends and magnitudes of a variety of MICP treatment schemes in half meter, one-dimensional flow columns. A design procedure is presented for predicting MICP in one-dimensional flow by sequentially coupling UCODE-2005 with TOUGHREACT.

1. Introduction

Until recently, research on microbial induced calcite precipitation (MICP) for geotechnical application has focused on characterizing strength, monitoring cementation, and optimizing treatment at small and large scales in laboratory and field experiments. MICP is a cementation process that harnesses natural subsurface bacteria using urea hydrolysis (ureolysis) to induce calcite precipitation at particle–particle contacts in soil environments [6,36,23]. MICP has been extensively evaluated for geotechnical ground improvement including increasing undrained shear strength [6,8], non-destructive geophysical monitoring [40,1], and solidification at laboratory and field scales [7,19,37,41,42]. MICP has also been identified as an engineering solution for a wide-range of disciplines including mineral plugging [11], environmental remediation of heavy metals [13], structural concrete repair [33,32,39], and carbon sequestration [35]. However, research to understand how MICP can be conceptually and quantitatively modeled is in its earliest stages.

Available mathematical modeling studies have addressed particular aspects of MICP including mechanical, hydro-geological, biological, and chemical processes. Many of the earliest studies focus particular attention to capturing the appropriate kinetic rates of ureolysis induced by single species and native microbes [12,18,24,25,26,15,13,14] as well as cell-free enzymes [16], and calcite precipitation [28]. Later studies evaluated the development of multi-component reactive transport by coupling similar ureolysis rate expressions to calcite precipitation kinetics and fluid transport in one- and two-dimensions [10,38,4,20,2]. A few studies have also examined the effects of reactive transport to mechanical changes in soil studies through finite element analysis [46]. Most of the models have been able to capture reaction rates for a variety of biological and chemical conditions within small-scale batch experiments via kinetic expressions accounting for chemical variants. There are needs to improve the quantitative modeling of MICP toward the coupling of constitutive theory from every involved discipline, and to improve the individual components for macro-scale reactive transport in porous media.

The study presented herein, builds from Barkouki et al. [2], implementing MICP into a bio-geo-chemical reactive transport code (TOUGHREACT; [43]) and calibrating unknown parameters (UCODE-2005; [31]) to verify the model and develop a procedure

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for predicting MICP in one-dimensional flow. The approach involves utilizing a suite of column experimental studies of MICP treatment to calibrate model parameters and predict calcite precipitation. Firstly, the model presented by Barkouki et al. [2] is optimized for calibration by adding weight factors to influence effectiveness of parameter convergence, using built-in sensitivity analyses and a high quantity of new experimental data. Secondly, a procedure for evaluating the model's predictive capability is presented by calibrating ureolytic activity rate prior to predicting spatially distributed calcite precipitate amounts under a variety of complex treatment schemes.

2. Experimental test program

The experimental data utilized for this study was extracted from the authors' previous work on the evaluation of MICP treatment in half-meter long column experiments. Detailed information related to methods can be found in Martinez et al. [22] while generally summarized here. The study considers five pairs of column experiments testing a variety of different treatment schemes in order to determine the best schemes for achieving uniform cementation over a half meter one-dimensional flow column. One set of column experiment data was presented in Barkouki et al. [2] and used for preliminary calibration of a MICP model by the coupling of UCODE-2005 to TOUGHREACT. To implement the joining of UCODE-2005 to TOUGHREACT for calibration. Two additional sets of column experiment data are used for this study, chosen for the complexity in their treatment schemes and high quality data.

Two acrylic columns (ID = 5.08 cm, OD = 5.72 cm, L = 60 cm) were fabricated with four evenly spaced locations along the length for two types of measurements: piezoelectric bender elements and fluid sampling ports (Fig. 1). Piezoelectric bender elements were utilized to send small-strain mechanical waves through the soil matrix to measure shear wave velocity in time and space during treatment [27]. Chemical analysis including pH, ammonium, and calcium was performed on samples extracted in space and time. Samples collected from the ports were either analyzed immediately (e.g. for pH) or stored at 4 °C for a maximum of 3 days before aqueous chemistry analysis. In some cases, microbe density was measured in space and time using spectrophotometry. Post-treatment calcite content was analyzed by dissecting the columns into approximately 20 discrete sections (sections associated with port locations tabulated) after treatment and acid washing samples to dissolve the calcium carbonate.

Various treatment schemes were used to evaluate MICP in the columns. A two phase treatment scheme was adopted for each column test including a bacterial treatment phase and a cementation treatment phase. The bacterial treatment phase involved augmentation of the bacterium *Sporoscarcina pasteurii* suspended in urea-rich solutions without calcium using a single pulse (high flow rate for a short time followed by longer retention time) or re-circulation (continuous circulation of fluid from outflow to inflow). The cementation treatment phase involved injection of urea- and calcium-rich solutions using stopped-flow or continuous flow (continuous feeding of injectate solution). In some cases, ureolytic potential tests (UPT) were conducted before initiation of the cementation treatment by injecting urea-rich solutions without calcium via a single pulse, followed by measurement of pH and/or urea in order to monitor the rate of ureolysis over the retention phase time associated with a typical stopped-flow cycle (one cycle includes the injection and retention phase). A summary of testing results is presented in Tables 1–3 for the two sets of column experiments used for this study.

Properties of the column related to the initial conditions (e.g. soil type, soil height, stress condition, porosity, shear wave velocity) and final shear wave velocity distribution are shown in Table 1. Ottawa 50–70 sand was air pluviated into columns to a relatively dense state and sand filters were used. Initial shear wave velocity profiles show higher velocities toward the top of the column (location D) where it is closest to the 100 kPa stress applied to the top and decreases with depth. The distribution in vertical stress along the column height is likely non-uniform given the influence of side

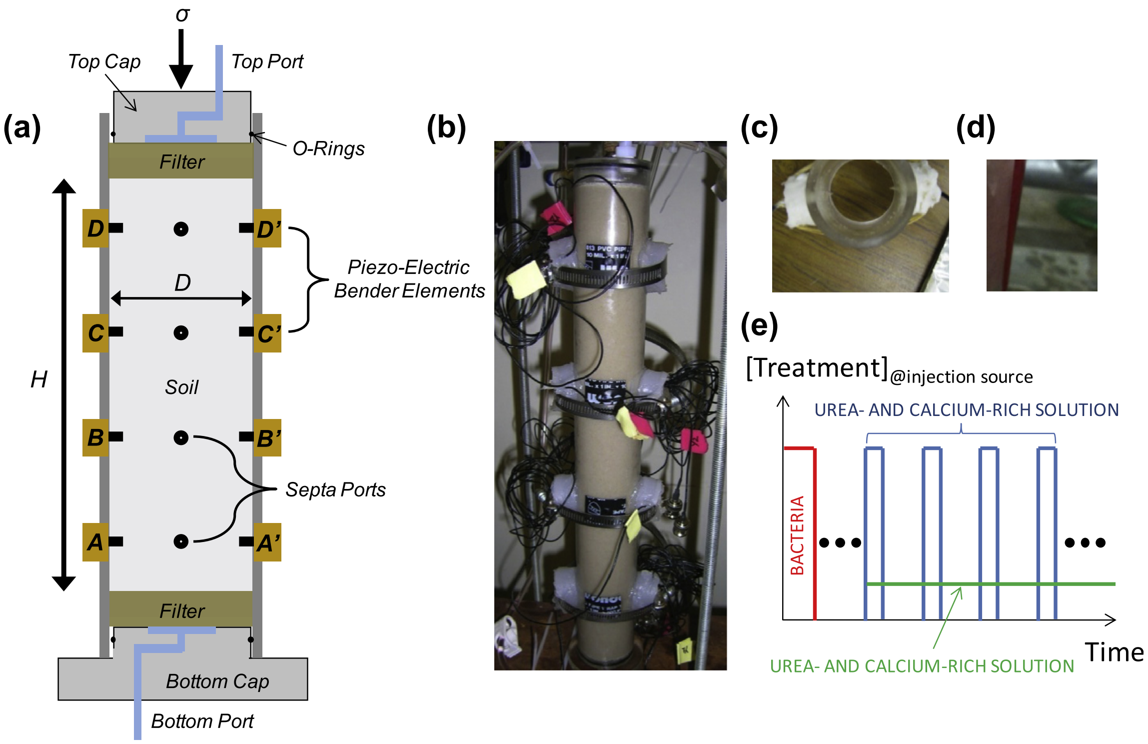

Fig. 1. Schematic diagram of half-meter column experiments, instrumentation, and treatment scheme.