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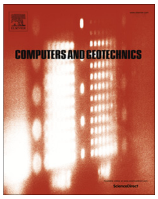

Research Paper

Discrete element method simulations of bio-cemented sands

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ABSTRACT

Microbially induced calcite precipitation (MICP) has emerged as a novel soil improvement method. In this paper, 3-D discrete element method (DEM) simulations are used to explore the behavior of MICP-cemented sands. Comparisons of the macro-scale response of numerical and physical specimens are made. Microstructure analyses indicate a shear band formed in the numerical specimens, consistent with physical experiments. The bond breakage pattern in numerical specimens is explored and compared to observed measurements from physical specimens. The relationship between dilatancy and stress-strain behavior is evaluated. The results indicate DEM is an effective technique to capture the mechanical behavior of MICP-cemented sand.

1. Introduction

The study of particulate micro-mechanics can provide important insights into the behavior of granular materials. Some microstructure experimental methods, such as resin-impregnation followed by digital image analysis (e.g., [33]), magnetic resonance imaging (e.g., [43]), and X-ray computed tomography (e.g., [57]), have been developed. However, these laboratory tests are difficult to perform, expensive and time consuming. The discrete element method (DEM), which was originally proposed by Cundall and Strack [10], is an effective simulation technique to provide insight into inter-particle forces and microstructure evolution. Of particular advantage to the current work, specimens with identical initial states can be used for tests under varying cementation levels and confinement. Furthermore, inter-particle information, such as meso-scale void ratio and coordination number, is accessible during any stage of the simulation.

Using DEM, many researchers have explored the behavior of clean sand under biaxial tests (e.g., [29]), triaxial tests (e.g., [9,3]), direct shear tests (e.g., [44,30,60]), and plain strain tests [53]. Particularly, Zhao and Evans [61] compared the mechanical properties of granular soils under triaxial, plane strain and direct shear loading states and concluded that DEM is capable of simulating varying loading conditions successfully without model recalibration.

Cementation, in either natural or artificial form, exists as an important improvement medium to strengthen soil static properties (e.g., [6,1,26,28,5]) and dynamic properties (e.g., [49,7]). Nevertheless, traditional artificial cementation media, such as Portland cement and gypsum, have limited injection distance due to high viscosity [52]. Recently, microbial induced calcite precipitation (MICP) has emerged as a new ground improvement strategy given its advantages of longer treatment distances and environmentally innocuous approach [13]. Taking advantage of urea hydrolysis catalyzed by a common soil bacteria *Sporosarcina pasteurii*, carbonate precipitation is created at soil grain contacts [14,41,4]. The improvement on soil properties through MICP has been verified by soil column tests (e.g., [59,37]), unconfined compressive tests (e.g., [47,50]), 1-D compression tests (e.g., [23,36]), triaxial tests (e.g., [14,40,24]), large scale laboratory tests (e.g., [56]) and in situ cone penetration test (e.g., [4]). Fauriel and Laloui [22] proposed a bio-chemo-hydro-mechanical model for bio-soil grouting application and made corresponding numerical examples. Although their model provides a good continuum solution to the coupled treatment in MICP processes, limited investigation is made on the mechanical response variation derived from MICP cementation.

Scanning electron microscopy (SEM) is able to provide evidence on the existence of calcite between soil particles when the specimen is dissected for analysis after shearing [15]; however, to the authors' knowledge, no insight can be obtained on the microstruc-

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ture evolution and bond breakage mechanism of MICP cemented soil under shearing, which is important to understand the macro-response of cemented soil. Using X-ray tomography, Tagliaferri et al. [54] observed localized deformation of MICP cemented sands during shearing and inferred cementation breakage pattern; while important, that work provides only qualitative information on the evolution of bond breakage rather than a robust quantitative analysis. Thus, it is beneficial to use DEM models to improve our understanding of the behavior and better inform the engineered design of bio-cemented sand, because these models can supply both qualitative and quantitative information on microstructure.

Furthermore, as mentioned above, although DEM of unbonded particles have been conducted by many previous researchers, the exploration on cemented sand is more limited (e.g., [58,16,20,11,12,45]), and always focused on chemical, rather than bio-mediated, cementation. Although an enhanced understanding of the mechanical behavior of cemented soil was provided by this prior work, it is not obvious that these results are applicable to bio-cemented sands, particularly when they are subjected to the full range of loading conditions applied in laboratory and field testing. A new bonding approach specifically tailored to DEM simulations of bio-cemented soils has recently been proposed [19,32], but this work is exploratory in nature and presently confined to simulation of relatively small particle assemblies.

In the current study, the response of MICP cemented sands from physical experiments are summarized, followed by the numerical model calibration corresponding to strength and deformation characteristics from physical experiments. Macro-response characteristics of the numerical specimens, and global void ratio and coordination number analyses are presented. Associated microstructure properties, such as mesoscale void ratio and coordination number, are analyzed in statistical and contour slices forms. Bond breakage patterns and evolution are captured for cemented physical specimens and related to the microstructure variation of the numerical specimens. Particularly, the bond breakage pattern evolution from the numerical model is compared to the bond breakage pattern from physical specimens, which is estimated using shear wave velocity measurements. The dilatancy characteristics and effect of cementation on soil behavior is discussed in detail.

2. Experimental procedure and results

The experimental MICP treatment process and the mechanical response of bio-cemented sands are summarized below. Traditional cementation media, such as Portland cement or gypsum, are normally applied by dry mixture with soil in the laboratory (e.g., [28]). MICP, which has a similar process to natural deposition [38], is gradually precipitated onto the sands grains and at the sand particle contacts. Ottawa 50–70 sand was selected as the sand matrix in this study. Index properties are summarized in Table 1.

Sporosarcina pasteurii (American Type Culture Collection, ATCC 11859) was the biological organism used to induce urea hydrolysis. To grow the bacteria to the desired population density, an ammonium-yeast extract media (ATCC 1376) was used. The growth media was inoculated with the *S. pasteurii* stock culture aerobically at 30 °C in a shaking incubator at 200 rpm for approximately 40 h before harvesting. Suspended culture after inoculation was then centrifuged at 4000*g* for 15 min. The supernatant was removed after the centrifuge period and replaced with fresh growth media. Finally, the desired bacteria were stored in the centrifuge vials at 4 °C until used.

Table 1
Sand characteristics.

D_{50} (mm)	C_u	C_c	G_S	e_{min}	e_{max}	Shape
0.22	1.4	0.9	2.65	0.55	0.87	Round

A two-phase injection procedure was used to induce cementation: in the first stage, suspended bacteria was injected through the specimen and retained in the pore space for at least six hours allowing for bacteria attachment; in the second stage, cementation media were repeatedly injected until the desired level of cementation was reached. A summary of chemical components and concentrations for the biological and chemical media is presented in Table 2.

Soil specimens were prepared by dry pluviation to a state with a similar initial global void ratio, approximately e = 0.72 (loose). To explore the effect of density, dense (e = 0.63) and medium dense (e = 0.70) specimens were also prepared. Complete details of the physical experiments can be found in Feng and Montoya [24]. Cemented samples were then confined under varying pressures (100 kPa, 200 kPa, and 400 kPa) and injected with cementation media to reach the target cementation levels. Once the cementation process was completed, backpressure saturation was conducted in order to obtain a B value greater than 0.95. The cementation content of specimens was finally determined by the acid washing method, after shearing under a rate of 2.5% per hour to a maximum axial strain of 25%.

Representative experimental results at a confinement of 100 kPa were selected to calibrate the numerical model. The experimental uncemented loose sand exhibits slightly dilative behavior, with shear stiffness, peak strength, strain-softening tendencies, and dilative volumetric strains increase with increasing density (Fig. 1). The experimental MICP cemented loose sand demonstrates a significant increase in initial stiffness, peak strength, and dilative volumetric strains compared to the loose uncemented sand (Fig. 2). Additionally, the peak strength of the MICP cemented specimens increases with an increase in cementation level. The experimental behavior is further presented in subsequent sections of the manuscript for comparisons to the simulated behavior. Detailed discussions of the experimental behavior can be found in Feng and Montoya [24].

3. Model and material properties

For comparison to laboratory results, three-dimensional DEM simulations were performed using PFC^{3D} [27]. Axisymmetric compression element tests were simulated on 2:1 H:D cylindrical assemblies of approximately 7000 particles with material properties similar to those of a clean quartz sand. The numerical model was first calibrated to uncemented sand behavior, as discussed subsequently. Initial conditions, boundary conditions, and model scaling were viewed to be of particular importance to the simulations and were considered in detail. Material and model properties are discussed in the following paragraphs and summarized in Table 3.

DEM simulations are typically comprised of two geometric entities: *balls* and *walls*. This makes the simulation of flexible membrane confinement, such as that used in physical triaxial experiments, challenging. Previous researchers have used strings of balls linked by contact bonds to simulate membranes in two dimensional simulations (e.g., [17,58,18]). A similar mechanism could be used in three dimensional models, but it increases the computational time significantly and is complex to implement. In the current study, stacks of cylindrical walls are used to simulate the flexible membrane [61], which saves computational time and allows the numerical membrane to deform independently since walls in PFC^{3D} do not interact with each other. Due to the frictional end platens in physical experiments, friction was also applied to top and bottom platens in the numerical specimens.