V International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2017
P. Wriggers, M. Bischoff, E. Oñate, D.R.J. Owen, & T. Zohdi (Eds)

A MODEL OF GRANULAR MATERIALS PARTIALLY CEMENTED BY BACTERIAL CALCITE

ELAHEH KASHIZADEH [1], ABHIJIT MUKHERJEE [2] AND ANTOINETTE TORDESILLAS [3]

[1]Department of Civil Engineering, Curtin University
Bentley WA 6102, Australia
E-mail address: Elaheh.kashizadeh1@postgrad.curtin.edu.au, URL: http://www.curtin.edu.au/

[2]Department of Civil Engineering, Curtin University
Bentley WA 6102, Australia
E-mail address: Abhijit.mukherjee@curtin.edu.au, URL: http://www.curtin.edu.au/

[3]School of Mathematics and Statistics, University of Melbourne
Victoria 3010, Australia
E-mail address: atordesi@unimelb.edu.au, URL: http://www.unimelb.edu.au/

Key words: MICP, Loose, Dense, Soil, Mechanical properties, DEM

Abstract. Nature aggregates granular materials such as sand, silt and clay into form beach rocks, anthills and other forms of microbialites. A common bio-geo-chemical cementation occurs due to the mineralization of calcium through bacterial enzymatic action, often called Microbial Induced Calcium Carbonate Precipitation (MICP). Unlike engineered cement, which consumes very high amounts of energy and emits large quantities of CO2, this natural cementation occurs in ambient conditions, with negligible energy consumption. Hence, it is a sustainable construction method. Natural cementation is a gradual process, where grains are initially bonded to form clumps. The clumps grow in size to form aggregates, finally creating free standing columns. Numerical models of the mechanical behaviors of cemented grains at the various stages of aggregation offer a way to explore and understand this process. In this paper, we propose a discrete element method (DEM) of aggregated granular materials formed due to MICP. The model is applied to study different levels of aggregation of sand, from sand heaps involving unbonded and bonded grains to free standing columns. The results are compared against experiments and the most important parameters are discussed.

1 INTRODUCTION

Granular materials such as sand, silt and clay are basic resources for construction. They are used in their natural unbonded forms such as earth embankments, and in bonded forms as in concrete. A binder, typically cement, is used to bond the grains together. The mechanism of resistance for loading in the loose and the bonded forms is fundamentally different. The loose material depends on the inter-granular friction for resistance against an applied force while the bonded material that behaves as a solid block has considerable inter-granular cohesion. A

numerical model that is able to capture all the stages of sand aggregation is challenging.

Presently, 3.6 billion tonnes per annum of Portland Cement is produced, contributing approximately 6% of all anthropogenic greenhouse gases [1]. Technologies that dramatically reduce or possibly eliminate Portland cement must be explored in order to improve the sustainability quotient of civil infrastructure. Recently, a new natural cementation, MICP, has been introduced as an alternative to cement binder [2]. In this process, bacterial enzymes are utilized to nucleate calcium carbonate as the cementing material [3]. Several important applications of the process is reported [4-6]. To optimize the process it is important to complement the experiments with a reliable numerical model. The model should be able to capture all phases of aggregation: from an assembly of loose grains to a free-standing assembly of fully aggregated (bonded) grains. In this paper, we propose a model of aggregated granular materials formed due to MICP using the discrete element method (DEM).

MICP is a bio-geo-chemical process that is performed to synthesise granular materials for a designed mechanical performance. Different aspects of the process, such as mass transport, bio-chemical reactions and consequent alternation in the mechanical response of the material have been modelled. Reactive transport models have been introduced to model biogrouting of soil [7, 8]. There have been attempts to simulate the bio-chemical process involved in MICP by solving transport and thermodynamic equations [9]. However, combining it with mechanical models is not reported hitherto. The mechanical property of sand columns resulting from MICP has been predicted using DEM [10, 11]. In these models MICP has been simulated as a homogenised cohesive system. However, the process can be highly localised, at least in the early stages. Moreover, a model of the mechanical response of a granular material from MICP at all levels of aggregation has not been reported.

The use of DEM for modelling granular materials dates back to Cundall & Strack [12]. The effect of non-idealized particle shapes on strength and deformation has extensively studied and one approach is by clustering idealized shape grains (e.g., circular disks and spheres)[13]. With the significant increase of computing power, discrete element models have been used to study the deformation of granular materials under a wide range of conditions in various fields including: geomechanics, pharmaceuticals, petroleum engineering, to name a few examples[14]. The present work is a first step towards the development of a DEM framework for modelling the mechanical behaviour of granular materials under MICP at all stages of aggregation. The model is applied to study the different levels of aggregation of sand, from sand heaps involving unbonded and bonded grains to free-standing columns. The results are compared against simulations and experiments and the most important parameters are discussed.

2 DEM MODELLING

In this study, a large complex granular system is considered as n-body structure of interconnected spheres. The center of each sphere is connected to the center of nearest contacted sphere(s). The connected lines create a complex network (Figure 1). Material constitutive properties are assigned to each connection.

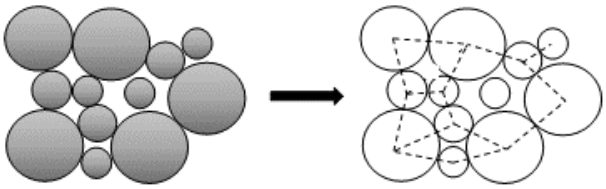


Figure 1: Relation between a granular material and a highly complex structural frame[15]

A spring–dashpot system is used for assigning the constitutive properties [11]. To simulate the contact forces between connected spheres; the spring, the divider and the dashpot model the contact force, the separation and damping . Figure 2 illustrates different spring-dashpot systems that are designed in numerical model to address normal, shear and rolling contacts.

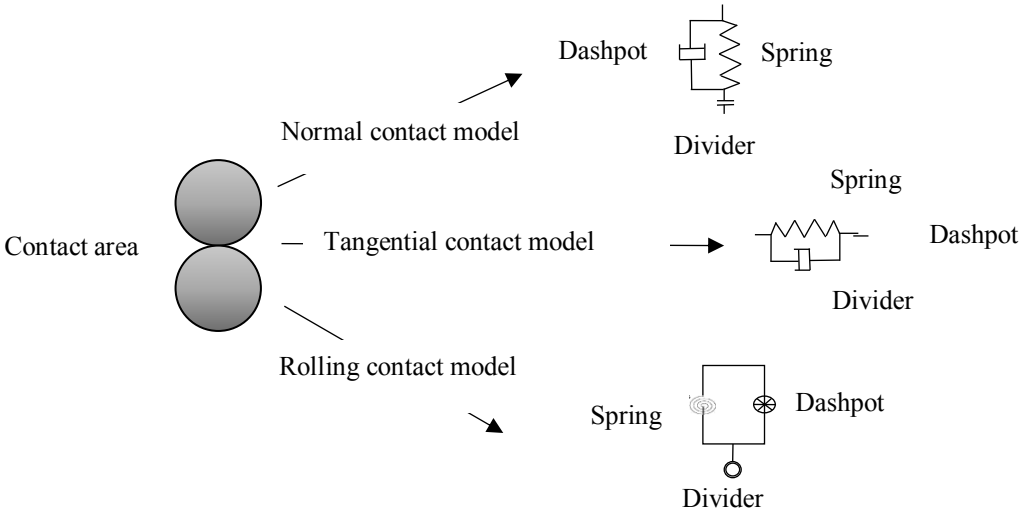


Figure 2: The contact models for grains with rolling resistance by Cundall [11]

A constitutive model with a combination of Hooke's and Coulomb's laws defines the interaction between the contacting particles:

$$f^n = k^n \Delta u^n + b^n \Delta \dot{u}^n \quad (1)$$

$$f^t = k^t \Delta u^t + b^t \Delta \dot{u}^t, for \left|\Delta u^t\right| < \mu \left|f^n\right| / k^t \quad (2)$$

Where:

f_n	Normal force component
f_t	Tangential force component
k^n & k^t	Spring stiffness coefficients
b^t & b^n	Viscous damping coefficients
μ	Coulomb friction coefficient
Δu^t & Δu^n	Relative normal and tangential displacement
$\Delta \dot{u}^t$ & $\Delta \dot{u}^n$	Relative normal and tangential translational velocities

The normal stiffness, k^n, shear stiffness, k^s and rolling stiffness, k^r parameters were calculated, as follows (Figure 2)

$$k^n = E_c \frac{2R_1R_2}{R_1 + R_2} \tag{3}$$

$$k^s = E_c v_c \frac{2R_1R_2}{R_1 + R_2} \tag{4}$$

$$k^r = \beta K^s R_1 R_2 \tag{5}$$

Where Ec is the Young modulus, vc is the Poisson ratio, R1 and R2 are the radii of the two connected spheres and β is the rolling stiffness coefficient. In the DEM model, by modelling the rolling resistance, I^c, the moments are introduced. The rolling resistance or contact moment—defined in an analogous fashion to Coulomb's law—is expressed as:

$$\begin{aligned} I^c &= k^r \Delta\alpha + b^r \Delta\dot{\alpha}, for \left|\Delta\alpha\right| < \mu^r R_{\min} \left|f^n\right| / k^r \\ I^c &= \mu^r R_{\min} \left|f^n\right|, for \left|\Delta\alpha\right| \geq \mu^r R_{\min} \left|f^n\right| / k^r \end{aligned} \tag{6}$$

Where:

R_{min} Minimum radii of the two interacting particles

k^r Rolling stiffness coefficients

μ^r Friction coefficient

$\Delta\alpha$ Relative rotation

$\Delta\dot{\alpha}$ Relative rotational velocities

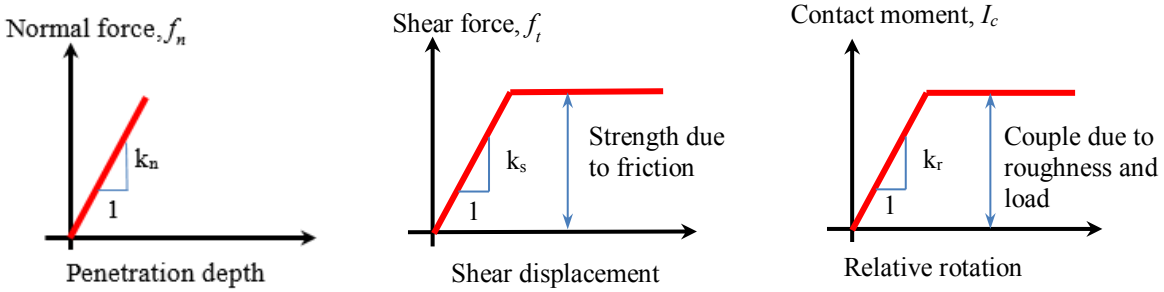


Figure 3: Mechanical stiffness of normal, tangential and rolling contact models[16]

Based on Mohr-Coulomb equation Figure 3 represents the mechanical response of normal, tangential and rolling contact model [17].

To solve the complex granular mechanism a numerical approach should be adopted [15]. In this paper an explicit finite difference, time-stepping algorithm, based on a Newton integration

equation, has been developed. The present numerical model is validated with experimental studies.

3 METHODOLOGY

To understand the mechanical behavior of granular materials a discrete element model (DEM) has been developed by using open-source discreet element software (YADE).To illustrate the capability of our numerical approach for modelling loose, semi- aggregated and fully aggregated samples, a series of investigations are carried out.

Numbers of spheres are created with specific grain size distribution in defined cubic format. Then property of material is assigned to spheres by defining the micro parameters. By controlling the number of grains and size of cube are the desired porosity is defined. The DEM models are closely calibrated to the initial configurations and packing densities of the experimental, as well as the contact and size distributions of the constituent particles.

3.1 Loose and Semi-aggregated Grains

In a loose or semi-aggregated state, the grains do not form a solid mass. Thus, they deform under the action of gravity and form a heap. When they are packed in a container and then the walls are removed, the grains move to form a heap. In the loose state, the grains are free to slide or roll over other grains once the intergranular friction is overcome. There is no cohesion between the grains. Partial aggregation is considered to be a state when some grains have bonded together due to MICP and formed a clump. Although the movement of the grains is prevented somewhat due to the formation of clumps, but the bonding is not wide spread so that the formation of heap under the action of gravity is prevented. The shape of the heap is dependent on the degree of aggregation. The semi aggregated state is modelled by rigidly connecting three grains together to create triads. The fraction of triads is proportional to the degree of aggregation. The shape of the heap is altered due to the formation of triads.

To illustrate the capability of our numerical approach to model this effect, a model has been developed in YADE. A cubic granular sample surrounded by walls is developed. All walls are removed simultaneously and the grains fall under the action of gravity. The released grains roll and slip on each other until their motion is below a set threshold. The threshold is set on the mean force magnitude of inter-particle interactions. Initially, there are a lot of movements, and the time progresses the particles stabilize into a shape resulting in negligible interaction forces. The tolerance value for this study for mean forces is 1e-2 Pa. In other words, the heap obtained when the mean interaction force drops below this threshold, all grains are considered static and the heap is considered to be the final configuration. A common assumption is that the shape of the heap will be conical and it can be represented by just the angle of repose. However, for semi-aggregated grains the shape of the heap is more complex and more parameters may be necessary to define the shape.

3.2 Aggregated Grains

In case of aggregated samples, the specimen retains its shape under the action of gravity. In addition to the frictional resistance against the relative motion between the grains, there is inter-granular cohesion due to the deposition of calcium carbonate at the grain intersections. The cohesive strength is dependent on the degree of MICP. As the samples are able to retain their shapes under the action of gravity, it is not necessary to contain them with the walls. Cylindrical samples have been developed with the specified grain size distribution. The samples have been

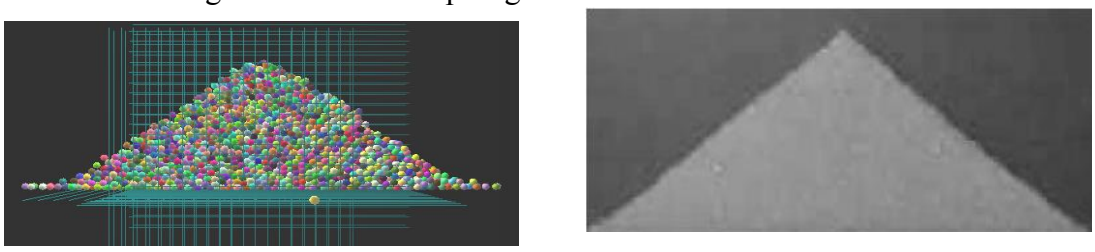
subjected to uniaxial compression at a constant rate until they collapse. In contrast to the previous case, in case of aggregated samples, the grains are tightly connected in the beginning. As a result, there is very little inter-granular movement, but as the load increases the inter-granular stress exceed the cohesive strength of MICP at a few locations resulting in cracking. As the cracking in the sample increases, the inter-granular movement also becomes more pronounced. As a result, the mean force magnitude of inter-particle interactions rises exponentially at the end of the numerical process indicating large inter-granular motions leading to collapse.

4 RESULTS

Results of simulation of grains aggregated in varying degrees by MICP using YADE is presented here. The aim is to validate the numerical observations with experimental results. The DEM simulation is controlled by the parameters described in (eqns. 1-6) that determine the inter-granular interaction (micro-parameters). It is not possible to have all these parameters measured experimentally. Thus, some of the parameters are adjusted to obtain the desired macro-parameters such as the angle of repose or the compressive strength.

4.1 Loose spherical glass bids

Zhou et al. [18] studied the angle of repose for mono-sized coarse spheres with 2mm diameter glass beads constrained by two glass walls separated by 40mm. The numerical model was developed by developing a container consisting of four glass walls with 80×8mm in pan and 40mm in height. The contained was filled with 2mm diameter glass bids. Then two smaller walls have been removed to allow flow of bids under the action of gravity. Flow through the shorter sides was allowed while the longer sides were rigidly constrained. The micro-parameters for the simulation are presented in Table 1 and the shape of the heap after 10000000 time steps is illustrated in Fig. 4. The angle of repose measured from the simulation and the experimentally observed angle are around 37°. Clearly, the present DEM model was able to model the stable configuration of the heap of glass beads.



(a) (b)

Figure 4: (a) The proposed numerical model in this study, (b) The experimental study by Zhou *et al*. [18], the angle of repose in both study is 37 degree

Table 1: The variables which have been considered for validation

Name of variable	Base value	Name of variable	Base value
Number of particles	2000	Density	2500 kNs2/m
Time step	10000000	Poisson ratio	0.3
Particle size	2 mm	Young's Modulus	2.16e6 Pa
Rolling friction coefficient	0.05	Damping	0.4
Sliding friction coefficient	0.5	Friction angle	22◦
Container thickness	40 mm		

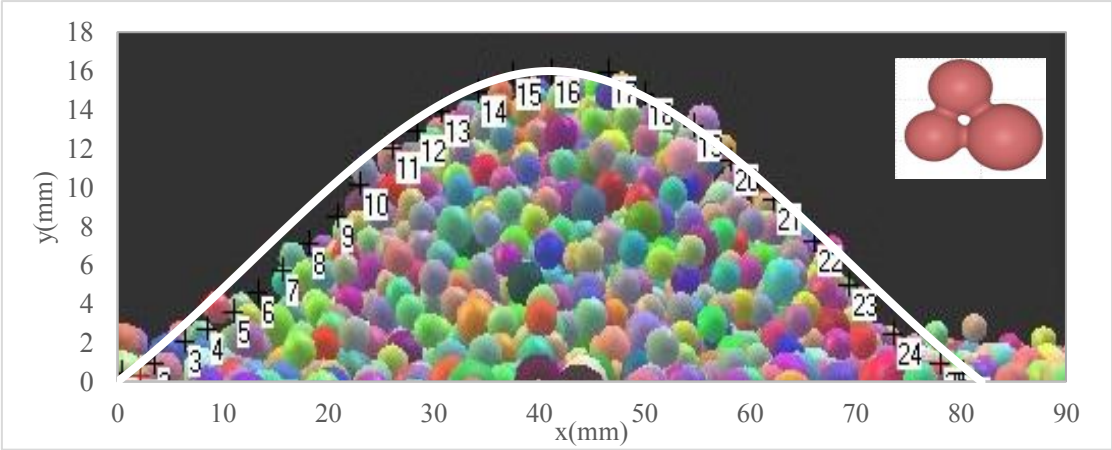
4.2 Semi-aggregated granules

To assess the intermediate situation, when a few grains have aggregated, but it is not enough to prevent the flow under the action of gravity, an experiment with a box of popcorns was conducted. The popcorns can approximate the shape of a triad where three spheres are clumped together signifying partial aggregation. A plastic container was filled with popcorns. The box was placed faced down on a firm table (Fig. 5a). Then the container was lifted suddenly. The popcorn takes the shape of a heap (Fig. 5b). The shape of the heap is noted by fitting a smooth curve to the contour of the heap.

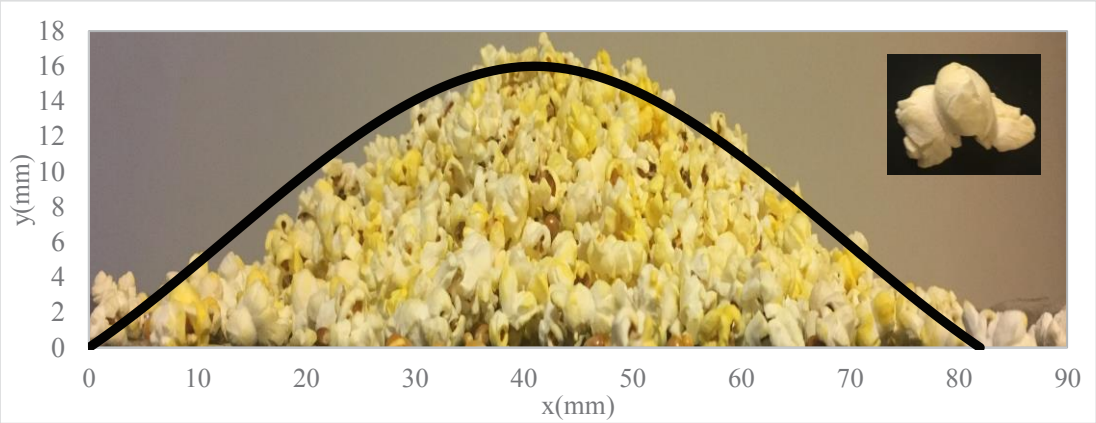
(a) (b)

Figure 5: Angle of repose study with pop-corn (a) pop-cons in container (b) accumulated shape of pop-corns after removing the container

The experiment has been simulated in a numerical model where the popcorn has been approximated as three spheres joined as a triad. The shape of the heap after 1e7 time steps is illustrated in (Fig. 6a) where the number of grains are 5000. A confined space of the same shape and size of the container is created by introducing four rigid walls. The confined space has been filled with the triads. Then the walls have been removed and the triads have been allowed to move until a stable configuration is reached (Fig. 6a). The shapes obtained from the experiment and the numerical model have been found to agree very well.



(a)



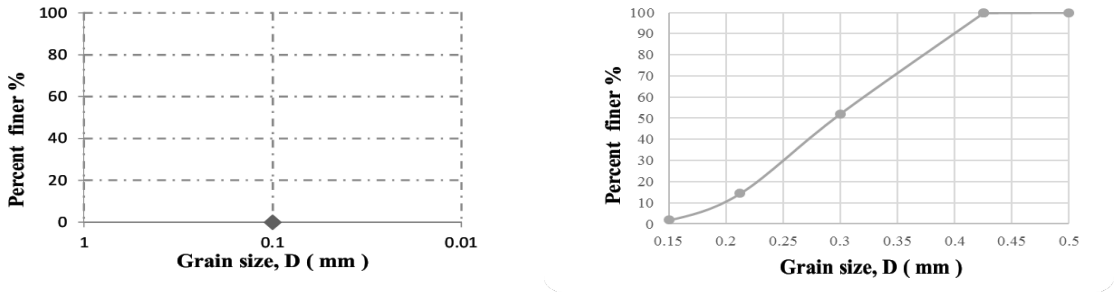
(b)

Figure 6: Comparison of Numerical model – the coloured grains have been used to make clumps distinguishable (a) and Experimental study (b) for semi-aggregated heaps, where the pop-cone grains shape is simulated as 3 spheres clumped

4.3Aggregated cylinders

Simulations of aggregated particles are validated with two experimental results at different extents of aggregation and particle size distribution. Jawad et al. [19] reported the results of unconfined compression tests of sand of single particle size (Fig. 7a) aggregated with MICP. While Porter et al. [20] reported MICP in well graded sand samples(Fig. 7b). Both samples were simulated in DEM and subjected to a displacement controlled unconfined compression test and the stress-strain curve for the sample has been plotted. It is important to set the micro-parameters for DEM to obtain a close fit with the experiments. The initial part of the curve is closely related to the elastic modulus of the grains. When the inter-granular stress exceed the strength of the cementation the grains start separating, sliding and rolling. Under these conditions the cohesion parameters play the most important role. Post-peak part of the stress-strain curve is dominated by the rolling stiffness and plastic moment limit strain.

Table 2 shows the values of parameters that are studied in the numerical approach to model the experimental of Jawad et al. [19]. Figure 8 illustrates the stress-strain curves from the numerical and experimental results. It can be seen that the two curves agreed overall. However, there are local differences between them. The initial slope of the numerical curve was considerably higher than that of the experiment. However, the slope reduced considerably between 2 and 4% strain and there was a good agreement at the peak stress and the strain at that instant. It is known that the samples created through MICP often have unevenness at their end surfaces, As a result, the initial slope is lower than expected as during the initial loading the uneven areas get gradually flattened resulting in more uniform distribution of stresses within the sample. The post-peak behavior of the samples was similar.



(a) (b)

Figure 7: Sand grain distribution to study Jawad *et al.* [19] , Porter *et al.* [20]

Table 2 Optimum values of micro parameters to model Jawad [19] experimental results

Name of variable	Base value	Name of variable	Base value
Number of particles	10000	Height of sample	80mm
Time step	1e7	Diameter of sample	37mm
Particle size	0.1 mm	Porosity	37.67%
Friction angle	36.5◦	Young modulus	17e6 Pa
Sliding friction coefficient	0.4	Normal cohesion	30e4 Pa
Density	2500 Kg/m3	Shear cohesion	9e6 Pa
Poisson ratio	0.4	Rolling stiffness coefficient	0.5
Damping	0.4	Plastic moment limit coefficient	0.15

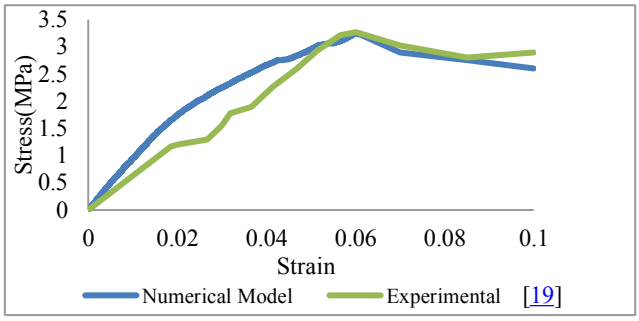


Figure 8: The stress–strain of the proposed numerical and experimental study [19]

The experiment reported by Porter et al. [20] has well graded grains. The samples have been given a lower level of MICP treatment resulting in intermediate level of aggregation, enough to have a cylinder but of lower strength than the previous example. The sphere packing technique is used to model the experimental samples to reach the porosity of sample around 36%. The parameters set in the DEM for this example are presented in Table 3. The stress-strain plots of the experimental and the numerical results are presented in Fig. 9. In this case too there was a good overall match between the experiment and numerical simulation. The initial apparent softness in the sample due to the unevenness of the loading surfaces is discernible in this experiment as well. The peak stress in the simulation occurred slightly later than that observed in the experiment. The post-peak behavior was captured well by the DEM. These examples demonstrate the capability of DEM in capturing the stress-strain behavior of

granular samples aggregated by MICP for a range of grain size distribution and extent of aggregation.

Table 3: Optimum values of micro parameters to model Porter *et al*. [20] experimental results

Name of variable	Base value	Name of variable	Base value
Number of particles	10000	Height of sample	60mm
Time step	1e7	Diameter of sample	30mm
Particle size	0.45 mm and 0.07 mm	Porosity	37.67%
Friction angle	36.5◦	Young modulus	17e6 Pa
Sliding friction coefficient	0.4	Normal cohesion	25e6 Pa
Density	2500 Kg/m3	Shear cohesion	6e3 Pa
Poisson ratio	0.4	Rolling stiffness coefficient	0.15
Damping	0.4	Plastic moment limit coefficient	0.15

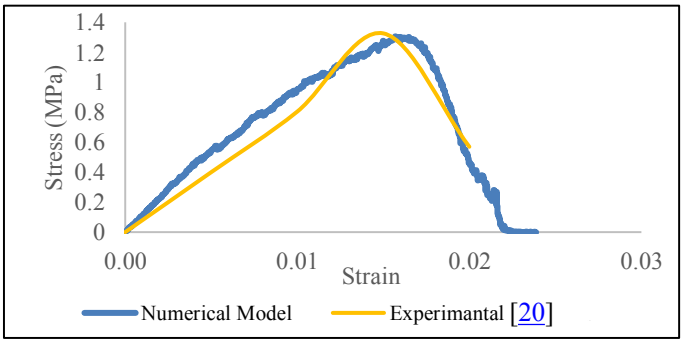


Figure 9: The stress–strain of the proposed numerical in current study and experimental study by Porter *et al*. [20]

We further explore the ability of DEM to identify cracks as they develop in the sample with the increasing load. Figure 10 shows the network of inter-granular distance for the grains on the surface of the cylinder. As cracks appear the grains that were initially cemented together separate when the stress in the cementation exceeds the cohesive strength. It can be noted that DEM predicts a developing vertical crack as the loading progresses. The red areas can be considered as separation as in those areas the distance between the grains has exceeded the average inter-grain distance at the beginning of the experiment. DEM predicts a vertical split failure of the sample. Fig. 11 presents the failure predicted by the DEM and that obtained in the experiment. There is a striking similarity between the two. Thus, it can be concluded that DEM is able to predict the failure mode of the Aggregated MICP samples.

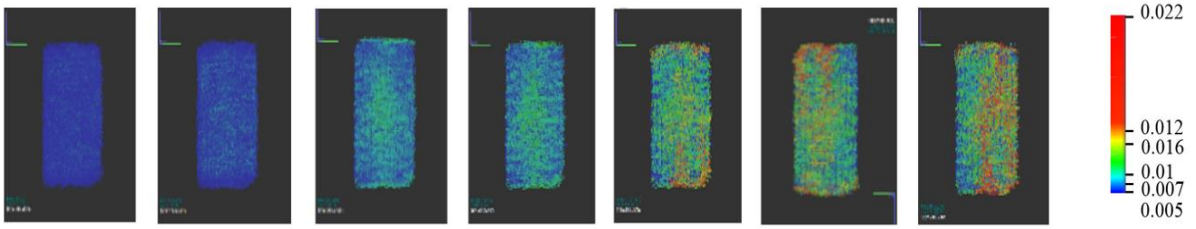


Figure 10: Inter-grain distances at different stages of the compression test on a highly complex structural frame where different colours are representing distance between grains, the blue is the smallest and red is largest distance– unit is mm

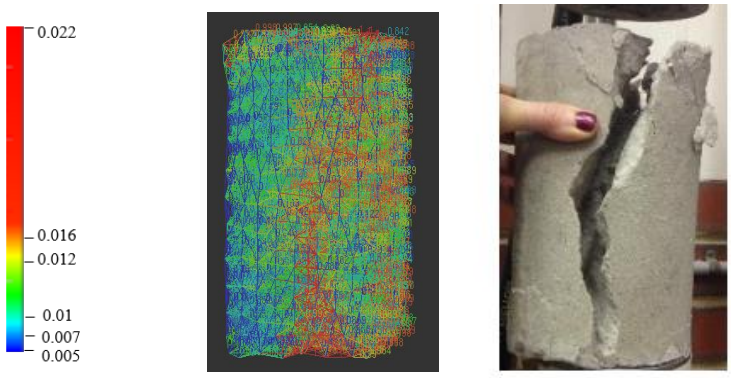


Figure 11: Comparison of failure modes obtained through the experiment and DEM simulation –unit is mm

6 CONCLUSIONS

This investigation explore the capability of DEM simulation for aggregation of grains by MICP to different extents. Comparing the series of simulation results with experiments the following conclusions can be made:

- Dem is able to model the aggregation of sand due to MICP at all the stages. The overall stress-strain graphs match well. However, the parameters of DEM must be set properly to get the best results.
- The shape of semi-aggregated heap can be modelled by clumping of grains to form triads.
- The stress-strain graphs of aggregated cylinders as obtained in the experiments can be emulated through DEM. However, the limit strength parameters such as cohesion and plastic moment limit have to be set properly.
- The inter-grain distance is a good measure for tracking cracks in aggregated cylinders. The failure mode predicted by the DEM was very close to that obtained in the experiment.
- The results of this investigation encourage us to explore the DEM modelling further for capturing MICP for a wide range of applications. A reliable numerical model would certainly expand the understanding of this exciting new technology for a wide range of applications.

7 REFERENCES

[1] Imbabi, M.S., C. Carrigan, and S. McKenna, Trends and developments in green cement and concrete technology. International Journal of Sustainable Built Environment, 2012. 1(2): p. 194-216.
[2] Achal, V., et al., Biomineralization for sustainable construction - A review of processes and applications. Earth-Science Reviews, 2015. 148: p. 1-17.
[3] Achal, V. and A. Mukherjee, A review of microbial precipitation for sustainable construction. Construction and Building Materials, 2015. 93: p. 1224-1235.
[4] Achal, V., A. Mukherjee, and M.S. Reddy, Microbial Concrete: Way to Enhance the Durability of Building Structures. Journal of Materials in Civil Engineering, 2011. 23(6):

p. 730-734.
[5] Achal, V., et al., Corrosion Prevention of Reinforced Concrete with Microbial Calcite Precipitation. Aci Materials Journal, 2012. 109(2): p. 157-163.
[6] Achal, V., A. Mukherjee, and M.S. Reddy, ORIGINAL RESEARCH: Biocalcification by Sporosarcina pasteurii using corn steep liquor as the nutrient source. Industrial Biotechnology, 2010. 6(3): p. 170-174.
[7] Laloui, L. and S. Fauriel, Birout propagation in soils.pdf. Multiscale and Multiphysics Processes in Geomechanics, 2011(SSGG): p. 77–80.
[8] Van Wijngaarden, W., et al., Modelling Biogrout: a new ground improvement method based on microbial-induced carbonate precipitation. Transport in Porous Media, 2011. 87(2): p. 397-420.
[9] Bouchelaghem, F. and L. Vulliet, Mathematical and numerical filtration-advection-dispersion model of miscible grout propagation in saturated porous media. International Journal for Numerical and Analytical Methods in Geomechanics, 2001. 25(12): p. 1195-1227.
[10] Yang, P., et al., 3D DEM Simulations of Drained Triaxial Compression of Sand Strengthened Using Microbially Induced Carbonate Precipitation. International Journal of Geomechanics, 2016: p. 04016143.
[11] Cundall, P.A., The measurement and analysis of accelerations in rock slopes. 1971, University of London.
[12] Cundall, P.A. and O.D. Strack, A discrete numerical model for granular assemblies. Géotechnique, 1979. 29(1): p. 47-65.
[13] Steefel, C.I., D.J. DePaolo, and P.C. Lichtner, Reactive transport modeling: An essential tool and a new research approach for the Earth sciences. Earth and Planetary Science Letters, 2005. 240(3): p. 539-558.
[14] Yeh, G.-T. and V.S. Tripathi, A critical evaluation of recent developments in hydrogeochemical transport models of reactive multichemical components. Water Resources Research, 1989. 25(1): p. 93-108.
[15] O'Sullivan, C., Particulate discrete element modelling. 2011: Taylor & Francis.
[16] Kozicki, J. and J. Tejchman. Numerical simulations of sand behaviour using DEM with two different descriptions of grain roughness. in II International Conference on Particle-based Methods–Fundamentals and Applications. Particles. 2011.
[17] Kozicki, J. and F. Donzé, A new open-source software developed for numerical simulations using discrete modeling methods. Computer Methods in Applied Mechanics and Engineering, 2008. 197(49): p. 4429-4443.
[18] Zhou, Y., et al., An experimental and numerical study of the angle of repose of coarse spheres. Powder Technology, 2002. 125(1): p. 45-54.
[19] Jawad, F. and J.-J. Zheng, Improving Poorly Graded Fine Sand with Microbial Induced Calcite Precipitation. 2016.
[20] Hannah Porter, N.K.D., Abhijit Mukherjee, Sustainable Road Bases with Microbial Carbonate Precipitation. SCMT4, Las Vegas, USA, August 7-11, 2016, 2016.