Three-dimensional DEM modelling of isotropic compression of cemented sand

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ABSTRACT

Isotropic compression tests were carried out on virtual cemented specimens with different values of cement content and initial void ratio by using three-dimensional (3-D) distinct element method (DEM), and the effect of cementation on cemented sands was examined. First, a simple 3-D bond contact model was introduced to represent the existence of inter-particle cementation. Second, a series of isotropic compression tests were conducted. Finally, the macro and micro-mechanical responses of cemented sands during loading were discussed. The results show that both cement content and density influence the compression curve of the cemented material. The macroscopic yielding is associated with bond breakage on microscopic scale. Bond breakage is primarily due to tension-shear and compression-shear failure, and occurs mainly in the strong contact force network. In addition, the bonded-contact orientation does not vary with compression pressure and cement content.

Keywords: cemented sand, distinct element method, isotropic compression, bond contact model

1. INTRODUCTION

The Both cemented and uncemented geomaterials are relatively incompressible at low stresses, and large volume changes only occur at very high stress levels in compression, leading to the well-known asymptotic states in the e-lgp plane, traditionally termed as normal compression lines (NCLs). For uncemented materials, particle crushing is always considered to be the dominant mechanism, while Mašín (2012) and Minh and Cheng (2013) propose that NCL is not related to grain crushing but caused primarily by particle rearrangement. Progressive bond breakage and particle crushing in cemented materials may account for the asymptotic states. Different from the NCLs for the uncemented materials, the existence of cementation in the cemented materials can increase the yield stress and allows the materials to exist in structure-permitted space (Leroueil and Vaughan 1990).

The available experimental data shows that the NCLs of cemented and uncemented materials either run parallel (Airey 1993; Do Santos Silva et al. 2010; Bobet et al. 2011; Rios et al. 2012) or converge (Cuccovillo and Coop 1999; Rotta et al. 2003). These differences may arise from sample preparation, material properties, or cementation constituent. Moreover, difficulty in sample repeatability definitely inhibits the experimental research. Alternatively, some authors attempt to investigate the compression behaviours of cemented materials by using DEM (Jiang et al. 2007; Jiang et al. 2013; de Bono and McDowell 2014). Similar to the experimental study, the aforementioned findings are reproduced. In their DEM studies, the adopted bond contact models are all developed based on assumptions, and do not take into account the influences of bond size, i.e., bond width and thickness, on the stiffness and strength envelops. In addition, the DEM simulations are primarily 2-D. In the 3-D simulation conducted by Bono and McDowell (2014), both cementation and grain crushing are considered, making the controversy more complicated. In this study, only the effect of cementation on the compression behaviours of cemented sands is focused.

2 BOND CONTACT MODEL

To represent the inter-particle cementation, a simple 3-D bond contact model has been developed based on the micro-mechanical tests on glued rods. The detailed information can be found in Ref. (Jiang and Zhang 2014; Jiang et al. 2014). In the following, a concise description on the contact model will be presented.

2.1 Contact force-displacement relationship

The contact model incorporates two typical types of bond model, i.e., the thin type and the thick type. Before the bond deposits, the force acting on the particles has been transmitted through particle contact in the thin bond model, but cannot be transmitted in the thick bond model due to the initial gap between particles. The normal displacement between particles, \( u_n \), is defined as the distance between the centers of the
two particles subtracted from the sum of their radius. The initial normal displacement, denoted as \( u_{n0} \), can be identified when the bond is formed.

For the thin bond model, the total contact forces are decomposed into two parts, i.e., one transmitted by the bond contact and the other transmitted by the particle contact.

\[
F_n = F_n^b + F_n^p, \quad F_s = F_s^b + F_s^p
\]  

(1)

where \( F_n, F_s \) are the normal and tangential contact forces, with superscripts \( b \) and \( p \) indicating the bond contact and the particle contact, respectively.

For the particle contact, its normal and tangential contact forces can be computed as:

\[
F_n^p = 0, \quad F_s^p = 0, \quad u_s < 0
\]  

(2)

\[
F_n^p = k_n^p \cdot u_n, \quad u_s > 0
\]  

(3)

\[
F_s^p = \min \{ F_n^p + k_n^p \cdot \Delta u_n^s, F_s^p + \mu F_n^p \}
\]  

(4)

where \( \Delta u_n^s \) is the relative incremental tangential displacement of the particle contact; \( \min\{\cdot\} \) is the operator taking the minimum value; \( k_n^p \) and \( k_s^p \) are the normal and tangential contact stiffnesses for the particle contact, respectively; \( \mu \) is the inter-particle friction coefficient.

The normal and tangential forces for the bond contact are expressed as follows.

\[
F_n^b = \begin{cases} k_n^b \cdot (u_n - u_{n0}), & -R_n^b \leq F_n^b \leq R_n^b \\ 0, & F_n^b < -R_n^b \end{cases}
\]  

(5)\(^b\)

\[
F_s^b = \begin{cases} k_s^b \cdot u_n^b, & \left( F_n^b / R_n^b \right)^2 \leq 1 \\ 0, & \left( F_n^b / R_n^b \right)^2 > 1 \end{cases}
\]  

(6)\(^b\)

where \( k_n^b \) and \( k_s^b \) are the bond’s normal and tangential contact stiffnesses; \( R_n^b, R_s^b \) are the bond tensile, compressive, and shear resistance, respectively; \( u_n^b \) is the accumulated tangential displacement since the bond contact is formed. Eqs. (5)\(^b\) and (6)\(^b\) show the failure criterion for bond. Specifically, if the force applied to a bond meets any one of the above conditions, the bond disappears and then cannot resist any forces.

For the thick bond model, only the bond contact resists the external load. In addition, the force-displacement relationship and the bond failure criterion in the thick bond mode are the same as those in the thin bond model, and are not described here for conciseness.

2.2 Bond strength

The formulas for the bond tensile, compressive and shear resistances can be written as follows.

\[
R_n^b = \sigma_n \times \pi \times \frac{B^2}{4} \times e^{-0.65 \ln \frac{B^2}{8D^2} \frac{B^2}{4} + \frac{1}{8D^2}}
\]  

(7)

\[
R_s^b = \sigma_s \times \pi \times \frac{B^2}{4} \times e^{-0.65 \ln \frac{B^2}{8D^2} \frac{B^2}{4} + \frac{1}{8D^2}}
\]  

(8)

\[
R_s^b = 0.37 \times e^{-0.65 \ln \frac{B^2}{8D^2} \frac{B^2}{4} + \frac{1}{8D^2}} \times \frac{E}{R_n^b + R_s^b} \times [1 - 2 \times \ln \left( \frac{R_n^b + R_s^b}{R_n^b + R_s^b} \right)]
\]  

(9)

where \( B, D \), and \( h_{\text{min}} \) are the width, diameter and the minimum thickness of bond; \( \sigma_n \) and \( \sigma_s \), i.e., the bond compressive and tensile strengths, can be calibrated by comparing the simulation results in the DEM tests and the experimental data in the laboratory.

2.3 Bond contact stiffnesses

The normal contact stiffness of bond for the thin bond model and the thick bond model can be ex-pressed as follows.

\[
k_n^b = 0.735 \times \ln \left( \frac{h_{\text{max}} - h_{\text{min}}}{R} \right) + 3.217 \cdot \frac{R \cdot E \cdot \pi \cdot B^2}{R} + h_{\text{min}} + B^2
\]  

(10)

\[
k_n^b = 0.735 \times \ln \left( \frac{h_{\text{max}} - h_{\text{min}}}{R} \right) + 3.217 \cdot \frac{R \cdot E \cdot \pi \cdot B^2}{R} + h_{\text{min}} + B^2
\]  

(11)

where \( h_{\text{max}} \) is the maximum bond thickness; \( E \) is the elastic modulus of bond; \( R = 2(r_1 r_2) / (r_1 + r_2) \) is the common radius, where \( r_1 \) and \( r_2 \) are the radii of two adjacent particles. In addition, the tangential contact stiffness of bond is assumed to be 0.5 times the normal contact stiffnesses for both bond models in this study.

In addition, the degree of cementation can be characterized following the concept of the critical bond thickness. As a result, the critical bond thickness \( h_{cr} \) used in the DEM study is 0.055 (0.0565), 0.0755 (0.078) and 0.091 (0.094) mm for the specimens with initial void ratio of 0.80 (0.85) and cement contents of 1%, 2% and 3% respectively. The detailed information can be found in Ref. (Jiang and Zhang 2014; Jiang et al. 2014).

It has been widely recognized that bond breakage is largely related to structural yield for cemented sand. To investigate the micro-mechanisms underlying the macroscopic yield of cemented sand, there are four
types of failure for bond considered in the above bond contact model, i.e., pure tension/compression, tension-shear and compression-shear failure. Specifically, tension (or compression)-shear means that the bond contact is subjected to both tension (or compression) and shear simultaneously. If a bond breaks due to tension (or compression)-shear, the failure type is defined as tension (or compression)-shear failure. The detailed information can be found in Ref. (Jiang et al. 2014).

### 3 ISOTROPIC COMPRESSION SIMULATIONS

The proposed contact model was implemented into PFC3D for simulating the isotropic compression tests on numerical cemented sands. The adopted material parameters used in the DEM simulations is summarized in Table 1. Two forms of damping are often used in most DEM simulations: viscous damping and local damping. Note that viscous damping and local damping have no significant effects in quasi-static behaviour, e.g. the isotropic compression behaviour of cemented sand investigated in this study. The viscous damping will be very useful in dynamic problems. However, as argued by Itasca (2004), the local damping has the advantage that only accelerating motion is damped, therefore no erroneous damping forces arise from steady-state motion. The damping coefficient is also non-dimensional and the damping is frequency-independent. Hence, local damping was used in this paper. A critical damping coefficient of 0.7 was chosen so that the particulate system is properly-damped while the viscous coefficient was set to zero so that the viscous damping was switched off.

Two cubic specimens with initial void ratio of 0.80 and 0.85 were first generated using the multi-layer under-compression method (Jiang et al. 2003). To prepare loose specimens, the inter-particle friction coefficient was set to 1.0. The resulted specimens were composed of spherical particles with radii ranging from 0.30 to 1.18 mm, forming a grain size distribution shown in Fig. 1. The specimens were compressed at the vertical stress of 12.5kPa until the equilibrium was reached. Bonds were then formed at the contacts where the gap between particles is smaller than or equals to the critical bond thickness $h_{cr}$, corresponding to a given cement content. In the isotropic compression tests, all six walls were movable and a set of pressures was applied identically on the specimens via these walls.

![Particle size distribution used in the DEM tests.](image)

### 4 SIMULATION RESULTS

To reveal the effect of density and cementation on the compression curves, a series of isotropic compression tests were conducted on virtual specimens of void ratio 0.80, 0.85 and cement content 1%, 2% and 3%.

Fig. 2 presents the influence of density on isotropic compression curves observed on the specimens of cement content 2% in laboratory and in the DEM tests. Like the experimental data on the uncemented sand, a reference curve obtained from the very-loose uncemented numerical material is also provided in the figure. Fig. 2 shows that the cemented numerical specimens exhibit several features as follows: (a) The void ratio of the cemented specimens is distinctly larger than that of the uncemented specimens; (b) For the cement content 2%, the NCLs for different densities tend to coincide with each other, and converge to that of uncemented material within the range of stresses analysed. This feature can also be found for other cement content shown in Fig. 3; (c) The pre-yield deformation is small, while volume decreases abruptly when the applied mean stress exceeds the yield stress. In addition, the yield stress increases with increasing of density.

It should be noted that the simulated reference curve differs from the experimental one. First of all, the former one was directly obtained from the very-loose material, while the latter one was obtained after the actual material yields. In addition, for the simulated reference, when the applied mean stress is less than 0.4 MPa, the void ratio decreases significantly. However, when the mean stress exceeds 0.4 MPa, the void ratio decreases slightly because the particle crushing which often occurs in reality is not considered in our simulations.

### Table 1. Material parameters used in the DEM simulations.

| Parameters                                | Value |
|-------------------------------------------|-------|
| Density/(kg·m$^{-3}$)                     | 2.650 |
| Compressive bond resistance/(MPa)         | 20    |
| Tensile bond resistance/(MPa)             | 1.0   |
| Elastic modulus of bond/(MPa)             | 4.0   |
| Normal contact stiffness of bond          | Eqs. (10) or (11) |
| Tangential contact stiffness of bond      | 0.5 × (Eqs. (10) or (11)) |
| Normal contact stiffness of particle/N·m$^{-2}$ | 1.5×10$^6$ |
| Tangential contact stiffness of particle/N·m$^{-2}$ | 0.75×10$^6$ |
| Friction coefficient between particles during loading | 0.5   |
| Friction coefficient between particle and wall | 0     |
| Local damping coefficient                 | 0.7   |
| Viscous damping coefficient               | 0     |
Fig. 2. Isotropic compression responses observed on specimens with different void ratio and cement content of 2%.

Fig. 3(a) provides the influence of cement content on isotropic compression curves for the DEM materials. Following the definition of primary yield proposed by Rotta et al. (2003), the primary yield points corresponding to variable cement content were identified in the figure. As shown in Fig. 3(a), the primary yield stress increases as cement content increases. Moreover, the NCLs for cemented materials converge to that for uncemented material. The available experimental and simulation results show that yield is associated with bond breakage (Rotta et al. 2003; Jiang et al. 2007). To investigate the underlying yielding mechanism, micro yielding is defined in terms of bond breakage (the largest gradient point on the Broken bond ratio-Mean stress curve), and the corresponding stress is the micro yield stress which does not equal to the tensile bond resistance. Fig. 3(b) presents the variation of broken bond ratio with the applied mean stress, where the micro yield points were marked. Like the primary yield point in Fig. 3(a), Fig. 3(b) demonstrates that the micro yield point can well be defined. When the applied mean stress is smaller than the micro yield stress, few bonds break; however, a large amount of bonds break once the applied mean stress exceeds the micro yield stress. In addition, comparison between Figs. 3(a) and (b) shows that the micro yield stress seems to be equal to the primary yield stress.

Fig. 4 presents the variation of bond breakage for the specimen with void ratio of 0.85 and cement content of 1%. The figure shows that bond breakage is primarily due to tension-shear and compression-shear. Moreover, the bond breakage occurs mainly in the strong contact force network. In the DEM modelling of 1-D compression of cemented sand conducted by Bono and McDowell (2014), it was found that the vast majority of bonds fail in shear rather than tension. However, they cannot determine whether the resulted bond breakage occurs due to tension-shear or compression-shear.

Figs. 5 and 6 illustrate the polar histograms of bonded-contact orientation within specimens with variable cement contents under different mean stresses. Due to the similar results for X-Z plane and Y-Z plane, only results on X-Z plane will be presented in the current study. It should be noted that the simulation results shown in Fig. 5 was calculated from the initial intact bond before the specimen was loaded. Both figu-
-res show that the contact orientation in the X-Y plane is isotropic, while that in the X-Z plane exhibits anisotropic behaviour, with the preference orientation along the vertical (Z) direction. Fig. 5 demonstrates that the area of polar histograms decreases as compression pressure increases due to bond degradation. In addition, both contact orientation in the X-Y plane and X-Z plane seem to be insensitive to compression pressure and cement content. When taken in combination, the data presented in Figs. 3, 5 and 6 again demonstrate that the differences in the compression curves is attributed to the degree of cementation, while not related to the bonded-contact orientation.

5 CONCLUSIONS

This paper presents a 3-D distinct element modelling of isotropic compression tests on virtual cemented sands. The following conclusions can be made from the investigation:

(1) The cemented specimens in the DEM tests exhibit the main features as those in laboratory. The NCLs for cemented specimens will converge to that for uncemented specimen.

(2) The primary yield is related to bond breakage. In addition, the primary yield stress seems equal to the micro yield stress.

(3) During the isotropic compression tests, the bond breakage is primarily due to tension-shear and compression-shear failure, and the bonded-contact orientation does not vary with the cement content and the applied compression pressures.

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