A novel and simple DEM simulation of unsaturated sand under fully undrained and compressible fluid condition

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ABSTRACT

This paper presents a new and simple method to investigate the unsaturated sand with a compressible fluid under undrained condition via the Distinct Element Method (DEM). In contrast to distinct element method and computational fluid dynamic approach (CFD-DEM) coupling, the pore pressure in this method is treated as the difference value between the initial confining pressure and the effective stress of the soil skeleton according to the effective stress principle. Furthermore, a compression coefficient is introduced to take into account the fluid compression, by which the changes of pore pressure and vertical strain rate of fluid can be calculated to control the movement of vertical walls. A series of three-dimensional (3D) cyclic simple shear tests were simulated to study the influence of fluid compressibility on the mechanical properties of soil. The DEM results were compared with the experimental data to verify the feasibility of the method.

Keywords: simple method, unsaturated sand, simple shear, compression coefficient, DEM

1 INTRODUCTION

The distinct element method (DEM) was firstly proposed by Cundall and Strack (1979) to simulate the mechanical behavior of granite by using a collection of particles that interact with each other. Since Thornton (2000) employed DEM to simulate the mechanical behavior of pure sands, more and more researches show that DEM is a powerful tool to simulate various complex soils including structured soils, loess, lunar soil, and to solve complicated geotechnical engineering problems including slope instability, soil bearing capacity and retaining walls.

It is well known that DEM is suitable to analyze dry granular materials. To analyze the liquefaction of saturated sand, two typical methods are usually employed: distinct element method and computational fluid dynamic approach (CFD-DEM) coupling method and constant volume method. The CFD-DEM coupling method has been widely used to study the multi-phase flow (Zeghal et al., 2008; Zhao et al., 2013; Jiang et al., 2014; Wang et al., 2017; Cheng et al., 2018). However, this method is computationally inefficient and many researches employed the constant volume method to simulate undrained test on the saturated material (Liu et al., 2007; You et al., 2017; Wei et al., 2019). In the constant volume method, the volume of sample keeps constant and the pore pressure is calculated as the difference of the effective stress on the side walls or within a measurement spine with initial confining pressure, in which the fluid is regarded as incompressible.

In comparison to saturated sands, unsaturated soil is more complex since it is a kind of three-phase assemble composed of solid phase (soil particles and some cementing substances), liquid phase (water and aqueous solution) and gas phase. The existence of the gas phase results in that the basic characteristics of unsaturated sand are different from those of saturated soil makes the mechanical and engineering properties complicated.

To date, efforts have been made to study the mechanical behavior of special unsaturated soils containing bubble soil (Wheeler, 1988; Pietruszczak et al., 1996, Wei et al., 2006), where the gas phase and the liquid phase are generally regarded as a compressive fluid. Thus the constant volume method becomes inapplicable for the unsaturated soil, while the CFD-DEM coupling method remains complicated and inefficient.

This paper aims to establish a novel and simple method of DEM to simulate undrained test on unsaturated sand with consideration of fluid compression. With the method, a series of three-dimensional (3D) cyclic simple shear tests were numerically carried out and the DEM results were compared with experimental data to verify the rationality of the simple method.
2 SIMPLE METHOD TO CONSIDER LIQUID COMPressIBILITY

In undrained test on unsaturated soil, the fluid will be compressed and its volume will decrease under loading. As a consequence, the total volume is not constant in the cycle simple shear test when the fluid compressibility is considered.

In order to consider the effect of fluid compression in undrained tests, the fluid compression coefficient (Liu et al., 2017) is employed to characterize the compressibility of the bubble. Thus, the reduction in the volume of fluid can be calculated based on the fluid compressibility and test conditions, which can be realized in the sample by changing the velocities of the boundary walls in DEM simulations.

The liquid compressibility can be expressed by:

\[ C_w = -\frac{1}{V} \frac{dV}{du} \]  

(1)

In the light that the mass keeps constant during the whole pressurization process, Eq. (1) can be rewritten as:

\[ C_w = \frac{1}{\rho} \frac{d\rho}{du} \]  

(2)

where \( V \) is the volume of fluid composed of bubbles and water, \( u \) is the pore pressure of fluid, and \( \rho \) is the density of fluid.

Therefore, a state equation of volume variation can be obtained as follows:

\[ \frac{\rho_f - \rho_{f0}}{\rho_f} = C_w (u_u - u_{u0}) \]  

(3)

where \( C_w \) is the compressibility of fluid. The compressibility of the bubble-containing pore fluid can be calculated by the following equation according to Liu (2017) when the surface tension is excluded:

\[ C_w = \frac{1}{V_{a0} + V_{w0}} \left( \frac{V_{a0}^2}{V_a^2} (u_{u0} + P_a) \right)^{-1} + S*C_{w0} \]  

(4)

where \( V_{a0} \) is the initial bubble volume, \( V_{w0} \) the initial water volume, \( V_a \) the current bubble volume, \( u_{u0} \) the initial pore pressure, \( P_a \) the standard atmospheric pressure, \( S \) the saturation, and \( C_{w0} \) the compression coefficient under the condition of saturation, which is 4.5×10^{-7} in this study.

Eq. (4) shows that the compressibility of fluid is a variable which depends on the saturation and bubble volume. Before simple shear test starts, the initial volume of the saturation and bubble can be measured in the sample to calculate the compressibility of fluid. Once the shear test begins, the incremental pore pressure \( \Delta u = u_u - u_{u0} \) will be updated by the difference between the initial pore pressure and the current pore pressure, which will then be used as initial pore pressure for calculation in next step. Thus, the compression coefficient of fluid \( C_w \) can be consequently updated with Eq. (4), and the volumetric strain of fluid \( \varepsilon_v^f \) can be calculated with Eq. (3).

The volumetric strain of the sample can be obtained by:

\[ \varepsilon_v = -\frac{\Delta V}{V_u + V_s} = \frac{V_u \cdot \varepsilon_v^f}{V_u + V_s} = \frac{\Delta h \cdot s_b}{V_u + V_s} \]  

(5)

\[ \Delta h = \frac{V_u \cdot \varepsilon_v^f}{s_b} \]  

(6)

where \( \varepsilon_v \) is the volumetric strain of the sample, \( V_u \) and \( V_s \) are the fluid volume and the soil skeleton volume, respectively. \( \Delta h \) is the vertical compression height composed of two equal displacement, and \( s_b \) the bottom area of the sample. In every step of the DEM simulation, \( \Delta h \) will be updated and applied to the top and bottom walls as shown in Fig.1.

3 DEM SIMULATION

3.1 Contact model and parameters

The contact model plays an important role in DEM simulations, which affects the reasonability of results. In order to take into account the effects of particle shape and surface roughness, the three-dimensional contact model incorporating rolling and twisting resistances (Jiang et al., 2015) is employed in this study. The model consists of four parts, i.e. the normal, the tangential, the bending rotation and twisting torsion components.

Table 1. Parameters of the contact model.

| Parameter                        | Value  |
|----------------------------------|--------|
| Particle modulus \( E_p \) (N/m²) | 3\times10^8 |
| Normal stiffness of each contact \( k_n \) (N/m) | 1.5\times10^7 |
| Shear stiffness of each contact \( k_s \) (N/m) | 1.0\times10^7 |
| Particle local crushing coefficient \( \xi_c \) | 2.1 |
| Rolling resistance coefficient \( \beta \) | 0.2 |
| Normal critical damping ratio \( \beta_n \) | 0.6 |
| Shear critical damping ratio \( \beta_s \) | 0.6 |
Table 1 presents the values of the parameters in the contact model, which were carefully calibrated to capture the mechanical behaviors of Ottawa 50-70 sand. More details can be referred to the thesis by Tan (2018).

3.2 Specimens

Ottawa 50-70 sand is the target in this DEM simulation, with a distribution of particle size shown in Fig. 2. The specimen modelled is composed of 48060 spheres with a maximum diameter of 0.524 mm, and a minimum diameter of 0.145 mm, an average grain diameter \( d_{50} = 0.33 \text{ mm} \) and uniformity coefficient \( C_u = d_{60}/d_{10} = 1.43 \).

The DEM sample was prepared using the multilayer with under-compaction method (UCM) (Jiang, 2003), since the method can generate a homogeneous sample efficiently. The sample was vertically compressed to a target void ratio of 0.73 with lateral and bottom walls fixed. The generated cubic sample has a side length of 9.38 mm.

The specimen was then pre-compressed under a vertical load of 12.5 kPa to reproduce a shallow, in situ stress state, which also exhibits inherent anisotropy prior to simple shearing.

4 NUMERICAL RESULTS

4.1 Macro-mechanical response

Fig. 3 provides the DEM results obtained from the cyclic simple shear test, presenting the relationship of shear strain vs stress, stress path, axial strain vs shear strain and evolution of compression coefficient. As shown in Fig. 3(c), (d), the axial strain and the compression coefficient increase in the initial stage of cyclic shearing, indicating the dilatant characteristics of sand.

In the cyclic shear process, the shear stress-strain demonstrates a hysteresis loop as shown in Fig.3(a). The stress path gradually moves towards the origin, as shown in Fig 3(b). The axial strain and the sample volume begin to decrease after reaching the peak. The peak of the compression coefficient starts to reduce gradually since the fluid is compressed cyclically, as shown in Fig. 3(c), (d). All those are in agreement with the results obtained from the DEM simulation (You et al., 2017) and laboratory test (Fakharian et al., 1997).

![Image](image-url)  
**Fig. 3.** The DEM results obtained from cyclic single shear test considering fluid compression: (a) stress-strain relationship, (b) stress path, (c) normal strain-shear strain relationship, (d) evolution of compression coefficient.

4.2 Mechanical coordination number and contact normal distribution

The mechanical coordination number is used to characterize the contact state between particles, which is defined by the following equation.

\[
C_n = \frac{2N_c - N_{b0} - N_{b1}}{N_b - N_{b0} - N_{b1}}
\]

where \( N_c \) and \( N_b \) are the number of total contacts and particles respectively, \( N_{b0} \) the number of particles with no contact, and \( N_{b1} \) the number of particles with one contact.

Fig. 4 presents the evolution of the mechanical coordination number in the cyclic simple shear test. It shows that the mechanical coordination number decreases rapidly from 4.00 to 3.73 at beginning. Then the...
mechanical coordination number tends to be change cyclically about a constant value of 3.71.

Fig. 4. Evolution of mechanical coordination number against shearing time.

Fig. 5 provides the contact normal distribution at different stages in the simple shear test, which reflects the evolution of the sample anisotropy. Note that the sample is isotropic before the test begins. In the first cyclic shearing process (Fig. 5(a), (b)), the distribution of contact normal rotates in accordance with the shear process in the x-z plane, which looks like a peanut instead of a circle. However, the distribution of contact normal changes little on the x-y and y-z planes. With the increasing of cyclic number, anisotropy becomes more obvious (Fig. 5(c), (d)).

5 CONCLUSIONS

This paper introduced a novel and simple method to simulate shear tests on unsaturated sand under undrained condition via DEM. With the method, a series of 3D cyclic simple shear tests were numerically carried out to demonstrate the rationality of the method. The stress-strain relationship, mechanical coordination number and contact normal direction were analyzed. The main conclusions can be drawn as follows:

1) The axial strain and the compression coefficient increase in the initial stage of cyclic shearing, indicating the dilatant characteristics of sand.

2) With the cycles number increase, the stress path gradually moves towards the origin, and the axial strain and the whole volume begin to decrease after reaching the peak, because fluid is compressed gradually.

3) The distribution of contact normal changes obviously on x-z plane in the shear process but changes little on the x-y and y-z planes.

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