Investigating the shear behaviors of unsaturated structured loess in direct shear test by the discrete element method

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\textbf{ABSTRACT}

This study investigates the shear behaviors of unsaturated structured loess in direct shear test by the discrete element method (DEM). A bond contact model characterized by the consideration of inter-particle attraction and van der Waals force was used. The direct shear tests were simulated under different suctions and vertical pressures. The simulation results were analyzed in terms of stress–strain relationships, volumetric responses, bond breakages and contact fabric. It is shown that: 1) The shear strength of structural loess samples can be enhanced by decreasing water content and increasing vertical pressure; the strain softening and dilatancy behaviors of structural loess enhance with the decrease of water content and vertical stress, respectively. 2) The bond breakage rate in shear band is related to the macroscopic mechanical response. 3) The anisotropy of the contact fabric changes more significantly in the shear band during shearing, it is of great significance to study the microcosmic properties of particles in shear band.

\textbf{Keywords}: unsaturated loess, direct shear test, DEM

\section{1 INTRODUCTION}

Generally, natural loess is aeolian soil, and the van der Waals force between particles cannot be ignored compared with particle gravity. Therefore, loess is prone to forming large pores during natural deposition. The strength of natural loess is high when the structure is intact. However, when it is affected by external forces, the cementation between grains will be destroyed, the mechanical properties of loess are changed, the loess will show collapsibility, and kinds of geological disasters could be induced, such as the development of ground cracks and vertical joints (Sun et al. 2009), the subsidence of buildings, structures and high-speed railway foundation (Derbyshire 2001). Therefore, the study of loess mechanics has been an important field of geotechnical research, with important theoretical and engineering significance for disaster prevention and reduction.

Direct shear test (DST) is a simple and effective method for determining of soil shear strength in laboratory. The sample will deform in the DST shearing process, accompanied with the rotation, slippage and fragmentation of particles. The deformation gradually develops and concentrates in the predetermined shear plane, which is usually referred to as the shear zone. The formation and evolution of shear zone lead to the instability and destruction of soil, which is a weak area that determines the strength of soil. Some laboratory tests on unsaturated loess have been carried out to study the shear strength (Shen et al. 2010; Zhang et al. 2016). These tests can reveal the macro-mechanical behaviours, however they are unable to analyse the relationship between the macro and micro mechanical responses of the sample. Moreover, the repeatability of the test is hard to guarantee.

The distinct element method (DEM), which was proposed by Cundall and Stack (1979), has unique advantages in the simulation of investigating the micro-mechanical performance of the soil. Great efforts have been made with DEM to study the mechanical properties of soils by DST. Thornton and Zhang (2003) simulated the DST on the grain; Liu et al. (2005) studied the direct shear properties of granular; Masson and Martinez (2005) comparatively studied the shear mechanical responses of loose and dense samples; Gutierrez and Wang (2010) investigated the size effect of the direct shear specimen by DEM. Jiang et al. (2010 a, b) studied the formation process of the shear band in the single-grain group dense sand and the formation mechanism and development process of sand shear zone through biaxial test. Li et al. (2017) studied the mesoscopic deformation mechanism of sand by simulating DST. Therefore, DEM has been widely used...
as an effective mean to analyse the macro and micro properties of soil. However, the mechanical properties of unsaturated structural loess under shear conditions are still unclear and need further studies.

In this paper, DEM was employed to simulate DST on unsaturated structural loess to study the macro and micro characteristics in DST with a reasonable micro contact model.

2 DEM SIMULATION

2.1 The contact model

A three-dimensional (3D) bond contact model proposed by Jiang et al. (2019) was used in this study. A unified adhesive force is incorporated into the rolling resistance model so that the influence of capillary force and weak attraction forces including van der Waals force can be considered. The model can be used to reproduce the mechanical properties of unsaturated loess, which has been applied to the lateral compression and wetting test of unsaturated loess (Li et al. 2018) and the isotropic compression tests of the unsaturated loess (Jiang et al. 2019).

2.2 Sample preparation

The spheres used in the simulation can capture the main features of loess grains and make the contact model as simple as possible. The 3D bond contact model was employed to simulate the cementing capacity between loess particles. This simulation method can simplify the simulation process and reflect the main mechanical characteristics of structural loess. Fig.1 provides the grain size distribution of the unsaturated structural loess in this study, where the median grain size is 20 μm. The DEM sample was generated with 40040 particles with the Multi-layer Under-compaction method (UCM) (Jiang et al., 2003) with a target size of 15.6mm× 15.6mm× 10.4mm, and the void ratio of sample is 0.84. To clearly show the characteristics during the shearing process, the assembly is coated with ten different colors along the x-axis (i.e., the shearing direction in Fig. 3). To investigate the particles in the shear band, a cube was set at the center of the sample, with 80 %, 40 % and 80 % of the width, height and length of the sample, respectively. An example of the generated sample is shown in Fig. 2.

2.3 Parameters of the sample

The particle parameters are provided in Table 1. The meaning and calibration of these parameters can be found in reference Li (2017).

2.4 DEM simulation scheme

After a sample was generated, it was firstly compressed one-dimensionally under a constant vertical pressure of 12.5kPa (pre-compression) to reproduce a shallow in situ stress state. After pre-compression, bonds were formed at the contacts, meanwhile the suction was set to different values to obtain the samples.

![Fig. 1. Grain size distribution.](image1)

![Fig. 2. Configuration of the DEM sample.](image2)

![Fig. 3. The measure spheres and applied vertical stress on the DEM sample.](image3)

| Table 1. Parameters of the DEM specimen. |
|-----------------------------------------|
| Parameter                                | Value |
| ---------------------------------------- |-------|
| Particle equivalent modulus, $E'$ (MPa) | 800   |
| The ratio of particle normal stiffness and tangential stiffness, $\kappa'$ | 1.5   |
| Inter-particle/particle-wall friction coefficient, $\mu$ | 0.5/0 |
| Inter-particle attraction coefficient, $\alpha$ (kPa) | 59.75 |
| Particle contact radius coefficient, $\beta$ | 0.3   |
| Equivalent modulus of cementation, $E''$ (MPa) | 200   |
| Modulus reduction factor, $\eta_S$ | 0.2   |
| The ratio of cementing normal stiffness and tangential stiffness, $k_b$ | 2.0   |
| Bonding strength, $\sigma_b$ (MPa) | 15    |
| Cementing tensile strength ratio, $\eta_a$ | 0.1   |
| Cementing radius coefficient, $\lambda_a$ | 0.35  |
| Cementing critical thickness factor, $g_c$ | 0.1   |
of different water content ($\omega$). Then they were consolidated one-dimensionally under a vertical stress of $\sigma_v = 50$, 100 and 200 kPa, respectively, and then sheared in the x-direction under a quasi-static condition. The sample was sheared by horizontally moving the upper and lower sections of the box in opposite directions at a speed of $V_x = 1\%$ /min, the global shear strain is defined as the displacement between the upper and lower sections divided by the sample length. Vertical stress ($\sigma_v$) was applied to the DEM sample through the top and bottom walls and kept constant by a servo control algorithm. As the purpose of this paper is to monitor the macro and micro characteristics of the structural loess in DSTs, two concentric measure spheres were set in the center of the sample, with their radii being 0.45 h (h is the height of the sample) for measure sphere 1 and 0.20 h for measure sphere 2, respectively, as illustrated in Fig. 3.  

3 DEM SIMULATION RESULTS

3.1 Macroscopic mechanical behavior

Figures 4(a) and 4(b) provide the stress–strain relationship and the evolution of void ratio obtained from samples with different water content and vertical stress. It can be observed that the shear strength of structural loess samples can be improved by decreasing water content and increasing vertical pressure. The strain softening and dilatancy behaviors of structural loess enhance with the decrease of water content and vertical stress, respectively. With the increase of vertical pressure, the samples are compacted in the compression stage, so that the yield strength and shear strength of the samples increase. The decrease of water content prevents the sample from being compacted in the compression stage, and only the capillary force and cementation strength can resist the shear stress. When the shear stress exceeds the resistance stress, the sample exhibits strain softening with the deformation and fabric restructuring.

Fig.5 provides the evolution of void ratio obtained from samples with the same water content at different vertical stress ($\sigma_v$). Measure sphere 1 was used to represent the whole sample, and measure sphere 2 was used to capture the feature of shear band. It can be clearly seen that there is a significant difference between the two measure spheres, indicating that the volume change is mainly caused by the change of particles in the shear zone. Therefore, the study of shear zone is helpful to explain shear mechanical properties of structural loess.

3.2 Cementation failure analysis

It is generally accepted that the formation of shear bands in cemented material is associated with bond breakage. To investigate this aspect, the relationship between bond-breakage rate and axial strain obtained from the samples is shown in Fig. 6. The bond breakage
The evolution of the contact fabric

Fig. 7 provides the granular fabric in the shear band of samples with $w=5.7\%$ at $\sigma_v=200$ kPa on the x–z plane during shearing. The fabric denotes the distribution of the directions of contact normal, and it is an important indicator of anisotropy. The granular fabric is obtained from all the grains in the shear band.

It can be observed that the anisotropy of the contact fabric increases significantly during the shear process, and it is more apparent in shear band than in whole sample. This indicates that the particles in the shear band underwent greater rotation during the shearing process. It is of great significance to study the microcosmic properties of particles in shear band.

4 CONCLUSIONS

This paper aims to study the macroscopic and microscopic mechanical properties of structural loess in direct shear test. A 3D bond contact model developed for unsaturated structured loess was employed. The multilayer under-compaction technique was employed to generate loose structural loess. A series of DSTs were carried out to analyze the stress–strain relationships, volumetric responses, bond breakage rate, and the evolution of the contact fabric. The main conclusions of the study are summarized as follows:

(1) The shear strength of structural loess samples can be enhanced by decreasing water content and increasing vertical pressure. The strain softening and dilatancy behaviors of structural loess enhance with the decrease of water content and vertical stress, respectively.

(2) Bond breakage starts at the material yielding point and reaches its maximum value during strain softening process. The bond breakage in shear band is related to the macroscopic mechanical response.

(3) The anisotropy of the contact fabric increases significantly during the shear process, and it is more apparent in shear band than in whole sample. It is of great significance to study the microcosmic properties of particles in shear band.

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