Comparison of Stress-Stain Behavior of CTC Test Using DEM Simulation

M. M. SAZZAD[1], E. SNEHA[2], R. B. ROUF[3]

[1]Department of Civil Engineering, RUET, Bangladesh (mmsruet@gmail.com)
[2]Department of Civil Engineering, RUET, Bangladesh (isratsniha@gmail.com)
[3]Department of Civil Engineering, RUET, Bangladesh (rownoak.rouf@gmail.com)

Abstract

Modeling the grain-scale behavior of granular materials using the discrete element method (DEM) has gained increasing attention to the researchers in the field of geotechnical engineering due to its advantages in exploring the mechanical behavior at grain-scale level. To warrant the behavior at grain-scale level, it is important to validate the DEM based macro-mechanical results with the experimental tests. This paper presents a comparison of the numerical simulation of the conventional triaxial compression (CTC) test by DEM with experimental studies. A numerical dry sample consisting of 9826 spheres was prepared by isotropically compressing the sample of randomly generated spheres with the periodic boundary and it was subjected to CTC test under strain controlled condition. The simulated stress-strain behavior agrees well to that of the experimental CTC test. The grain-scale quantity has been correlated with the macro-scale quantity and a linear macro-micro relationship is noticed.

Keywords: *Numerical Simulation, Grain-Scale Behavior, Discrete Element Method.*

1 Introduction

Granular material such as sand is often modelled with the continuum concept by using the finite element method (FEM). However, the models using the continuum mechanics are phenomenological and do not consider the fundamental physical significance of a particulate system. Practically, the loads in a granular system are transferred by interparticle contacts. This inherent granulate nature of granular materials is not included in modeling the behavior of granular system in continuum mechanics which cannot capture the actual deformation and failure modes of such system. This inherent discrete nature makes the development of constitutive laws very complex and many physical tests are necessary to understand the physical processes before devolving a constitutive relation. This limitation in continuum modeling by FEM makes the discrete element method (DEM) so popular now-a-days and it draws the attention of numerous researchers in the field of geotechnical engineering (e.g., Antony et al., 2004; Ng, 2006; O'Sullivan et al., 2008; Sazzad and Suzuki, 2011; Kuhn et al., 2014; Perez et al., 2016). Moreover, the internal physical processes in a sample cannot be explored and understand by using the FEM modeling. Consequently, the physical processes that lead to the failure of a granular system cannot be explained using the continuum models and DEM must be used. In the DEM modeling, the qualitative comparison of the simulated result is often used. The qualitative comparison of the DEM based results with the experimental studies is valid as long as the behavior of granular material such as sand at grain-scale level is of the major interest of the study. However, to warrant the behavior at grain-scale level, it is also important to compare the DEM based simulated results with the experimental studies.

In the literature, very few studies were reported that compared the simulated results of CTC test using the DEM with the laboratory based experimental studies. For example, Suiker and Fleck (2004) reported a triaxial tests on an aggregate of steel sphere and compared the mobilized friction angle at residual state for different interparticle friction angles with the DEM simulations. Cui et al. (2007) conducted a CTC test on dry Grade chrome steel balls under vacuum confinement of 80 kPa Even though few studies were reported in the literature, the macro-micro relationship is not established after the quantitative comparison of the experimental results with the DEM simulations. Consequently, the aim of the present study is to compare the simulated results of CTC test by DEM under strain controlled condition with the experimental study qualitatively and to propose a macro-micro relation. A virtual dry sample consisting of 9826 spheres was prepared by compressing the sample of randomly generated spheres isotropically with the periodic boundary, a boundary condition in which the periodic cells are surrounded by the identical cells. The generated numerical sample was compressed in different stages to attain a confining pressure of 80 kPa. A deformation rate tensor was used to apply the global deformation uniformly. The isotropically compressed numerical sample was subjected to CTC test under strain controlled condition and the simulated macro result was compared with that of the CTC test. The grain-scale quantity such as the fabric is measured and the relationship between the macro quantity (normalized deviatoric stress) and the grain-scale quantity (fabric ratio) has been established.

2 About DEM and OVAL

Discrete element method (DEM) is a numerical technique proposed by Cundall and Strack (1979) for modeling the discrete behavior of granular materials. The particle considered in DEM can move and rotate through the interactions of the interparticle contacts. The translational and rotational accelerations of a 3D particle in DEM are calculated following the Newton's second law of motion which can be expressed as follows:

$$m\ddot{x}_i = \sum F_i \qquad i = 1-3 \tag{1}$$

$$I\ddot{\theta} = \sum M \tag{2}$$

where F_i are the force components, M is the moment, m is the mass, I is the moment of inertia, $\ddot{x}_i$ are the translation acceleration components and $\ddot{\theta}$ is the rotational acceleration of the particle. The accelerations are integrated twice over time to obtain the displacements. For details of DEM, readers are referred to Cundall and Strack (1979).

In the present study, computer program OVAL (Kuhn, 2003) is used. It is a program written in FORTRAN language and runs on both Windows and Linux platform. It is used for analyzing the particulate assemblies using DEM (Cundall and Strack, 1979). It includes a robust servo-control algorithm to control the boundary stresses. It has been used for many DEM based studies so far and its effectiveness has been recognized (e.g., Kuhn, 1999; Sazzad and Suzuki, 2010; Sazzad, 2014). In present study, Hertz-Mindlin contact model is used. The normal force of a Hertz-type contact is computed as follows (Kuhn, 2006):

$$F^n = \frac{\overline{E}a^3}{R} \tag{3}$$

$$\overline{E} = \frac{8G}{3(1-\nu)} \tag{4}$$

$$a = \sqrt{\frac{d \times R}{2}} \tag{5}$$

$$R = \frac{2R_1R_2}{R_1 + R_2} \tag{6}$$

Here, $\overline{E}$ is the elastic constant, a is the contact radius, d is the overlap between the contacting particles, R is the effective radius of curvature, R_1 and R_2 are the radii of curvatures of two particles at contact.

3 Brief Description of the CTC Test

In the present study, the laboratory based triaxial test (CTC test) reported in Cui et al. (2007) and O'Sullivan et al. (2008) on dry Grade chrome steel balls under vacuum confinement of 80 kPa has been followed. The nonuniform sample in their study had three types of spheres of radii of 2 mm, 2.5 mm and 3 mm, respectively. The mixing ratio of these spheres for nonuniform sample was 1:1:1 with a sample height to width ratio of two. The void ratio of nonuniform sample was 0.603. The characteristics of the spheres used in the CTC tests as reported in Cui et al. (2007) and O'Sullivan et al. (2008) have been summarized in Table 1. The interparticle friction coefficient and the boundary–particle friction coefficient were measured by O'Sullivan et al. (2004) and Cui (2006). For details of the laboratory based CTC test, readers are referred to Cui et al. (2007) and O'Sullivan et al. (2008).

Table 1. Characteristics of dry Grade chrome steel balls used in the CTC test (after Cui et al., 2007)

Properties	Values
Density of spheres (kg/m^3)	7.8 ×10^3
Shear modulus (Pa)	7.9 ×10^3
Poisson's ratio	0.28
Interparticle friction coefficient	0.096
Boundary friction coefficient	0.228

4 Preparation of Numerical Sample

4.1 Sample Generation

A numerical sample consisting of 9826 spheres has been randomly generated such that each sphere is not in contact with any of its neighbor. The spheres have been modeled as the particles. This is because it simplifies the contact detection among spheres and therefore, it reduces the computational cost of the simulation. Moreover, the primary goal of the present study is to compare the simulated results of virtual triaxial test with the similar laboratory based CTC test reported in Cui et al. (2007) and O'Sullivan et al. (2008), where the steel balls (i.e. spheres) were used. The centers of the spheres have been placed in the grid points of sample. Three types of spheres have been considered in the present study following the CTC tests reported in Cui et al. (2007) and O'Sullivan et al. (2008). The radii of spheres are 2 mm, 2.5 mm and 3 mm, respectively. The mixing ratio of spheres is 1:1:1 as has been reported in Cui et al. (2007) and O'Sullivan et al. (2008). During the generation of the numerical sample, the spacing of the grid is equal to the maximum radius of the sphere to ensure that no sphere can overlap the others. The initial sample generated in this way is very sparse and needs to be compressed isotropically. The initial sample is surrounded by the periodic boundaries, a boundary condition in which the periodic cells are surrounded by the identical cells.

4.2 Preparation of Isotropically Compressed Sample

The generated numerical sample has been compressed in different stages to attain a confining pressure of 80 kPa. During the compression, the periodic boundary condition is applied similar to that used in the conventional DEM based study. A particle that sits astride a periodic boundary has a numerical image at the opposite boundary. If the centers of the particles move outside one circumferential boundary, they are immediately reintroduced at a corresponding location along the other circumferential boundary. The consolidation of the initially generated sparse sample has been carried out using the strain controlled condition. A deformation rate tensor is used to apply the global deformation uniformly. The volume of solids is computed by adding the volume of individual particle and the volume of void is calculated by subtracting the volume of solids from the total volume of sample. The void ratio is measured by dividing the volume of void by the volume of solids. After the end of isotropic compression, the void ratio of the numerical sample becomes 0.626, which is very close to that found in the CTC test for non-uniform sample. Note that, only non-uniform sample is considered in the present study to compare the DEM simulation of triaxial test with the CTC test.

5 Numerical Simulation of CTC Test

The simulation of the CTC test has been carried out under the strained controlled condition using DEM. A very small strain increment is assigned so that the quasi-static condition is attained and the effect of numerical damping becomes minimum. To monitor the quasi-static condition, the non-dimensional index I_{uf} is defined as follows (Sazzad, 2016):

$$I_{uf} = \sqrt{\frac{\sum_{1}^{N_p} F_{ubf}^2 / N_p}{\sum_{1}^{N_c} F^2 / N_c}} \times 100(\%), \tag{7}$$

where F_{ubf}, F, N_p and N_c denote the unbalanced force, contact force, number of particles and number of contacts, respectively. Index I_{uf} is directly related to the accuracy of the simulation. Lower the value of I_{uf}, higher the accuracy of the simulation. The material properties and DEM parameters used in the simulation is shown in Table 2. Note that the material properties of the DEM simulation are same as that of grade chrome steel balls used in the CTC test.

Table 2. Material Properties and DEM parameters used in the present study

Properties	**Values**
Density of spheres (kg/m^3)	7.8 ×10^3
Shear modulus (Pa)	7.9 ×10^3
Poisson's ratio	0.28
Interparticle friction coefficient	0.096
Increment of time step (s)	1.0 ×10^{-6}
Damping coefficients	0.10

6 Comparison of DEM Results with the CTC Test

The Simulated stress-strain behavior is compared with the laboratory based CTC test as reported in Cui et al. (2007) and depicted in Figure 1. The normalized deviatoric stress is defined here as $\sigma_d = (\sigma_1 - \sigma_3)/\sigma_3$, where σ_1 and σ_3 are the stresses in vertical and lateral directions, respectively. Note that the simulated stress-strain behavior carried out by DEM is in excellent agreement with the laboratory based CTC test under strain controlled condition. This quantitative validation of the simulated results with that of the experiment depicts the versatile nature of the present study by DEM and proofs that DEM can successfully replicate the behavior of granular materials even quantitatively. The relationship between the axial strain and the lateral strain is also depicted in Figure 2. Note that no comparison is shown (Figure 2) between the simulated results and the experimental results because the relationship between the axial strain and the lateral strain was not reported in Cui et al. (2007) and O'Sullivan et al. (2008).

7 Macro-Micro Relationship

The relationship between the macro quantity (normalized deviatoric stress) and the grain-scale quantity (fabric ratio of strong contact) is depicted in Figure 3. The contact fabric considering only the strong contacts is quantified using the following tensor (Sazzad and Suzuki, 2013):

$$H_{ij}^s = \frac{1}{N_c}\sum_{s=1}^{N_s} n_i^s n_j^s \qquad i,j = 1-3 \tag{8}$$

where, n_i^s is the $i-$th component of the unit contact normal vectors at the $s-$th strong contact. A contact is said to be a strong contact if it carries a contact force greater than the average contact force (f_a) defined as follows (Sazzad, 2016), where f^k is the contact force at $k-$th contact.

$$f_a = \sqrt{\frac{\sum_{k=1}^{N_c} \left|f^k\right|^2}{N_c}} \tag{9}$$

The deviatoric fabric for strong contact are defined here as follows:

$$H_d^s = (H_{11} - H_{33})/H_{33} \tag{10}$$

It is noted that a linear macro-micro relationship exist between the normalized deviatoric stress and the deviatoric fabric. The relationship between the micro-quantity (fabric ratio) and macro-quantity (normalized deviatoric stress ratio) can be given by the following equation:

$$H_d^s = 1.35\sigma_d \tag{11}$$

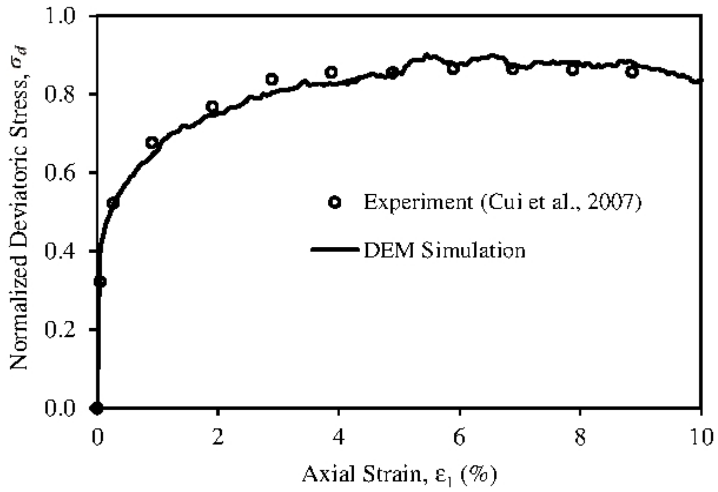

Figure 1. Comparison of the simulated stress-strain behavior with the CTC test (experiment) reported in Cui et al. (2007)

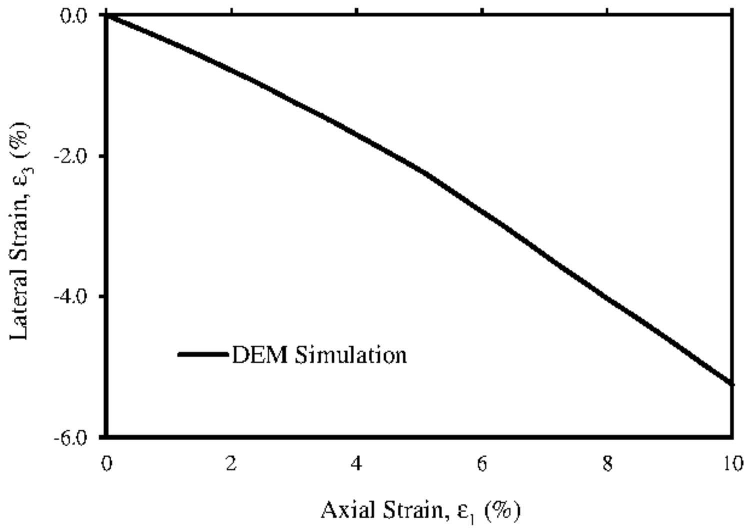

Figure 2. Relationship between the axial strain, ε_1 and lateral strain, ε_3 during the simulation

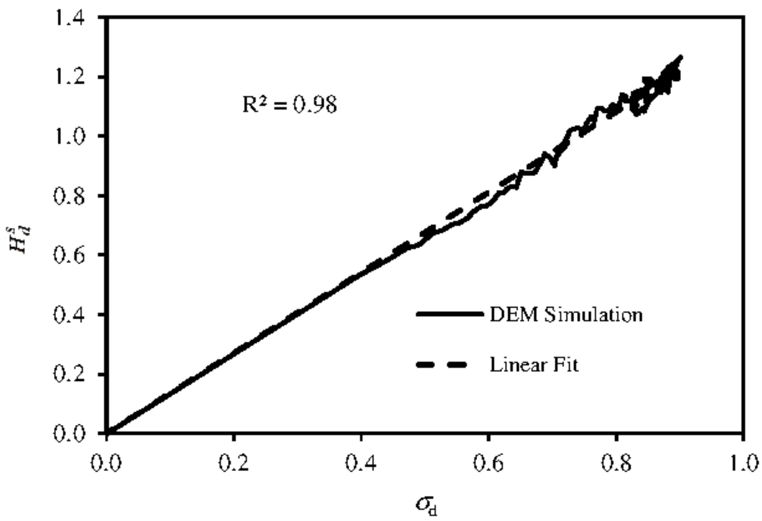

Figure 3. The relationship between the micro-quantity (fabric ratio) and macro-quantity (normalized deviatoric stress ratio) during the simulation

8 Conclusions

The present study aims at comparing the simulated behavior of granular materials by DEM with the laboratory based CTC test quantitatively. A numerical dry sample consisting of 9826 spheres was subjected to CTC test under strain controlled condition. The findings of the study can be summarized as follows:

i. The simulated stress-strain behavior using the DEM agrees well quantitatively to that observed in the CTC test reported in Cui et al. (2007). This demonstrates the worth and reliability of the present simulation by DEM.
ii. A linear macro-micro relationship exists between the normalized deviatoric stress and the fabric ratio when strong contacts are considered in quantifying the fabric tensor.

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