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Effect of sample size on the macro and micro-scale behaviour of granular materials using 3D DEM

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Abstract: This paper presents the effect of sample size on the macro- and micro-scale behaviors of granular materials such as sand using the three-dimensional (3d) discrete element method (dem). Three numerical samples of different sizes were prepared using spheres as particles. During the random sample generation, spheres of different radii were placed randomly in a cube without any contact. After the random generation of three successful samples, they were subjected to isotropic compression by moving their boundaries inward. Simulations of true triaxial compression tests were carried out using these samples to investigate their behaviors both at macro- and micro-scale. The numerical results indicate that the tress-strain-dilative behavior agrees well with the laboratory based experimental results qualitatively for different sample sizes. Small size sample attains the highest strength and it decreases as the sample size increases. It is noted that the evolution of coordination number is the highest for small size sample and it decreases as the sample size increases.

Keywords: *Sample Size, Micro-Scale, Granular Materials, Simulations*

1. Introduction:

Sample size is known to have influence on the mechanical behaviors of granular materials such as sand, both at macro- and micro-scale. The sample size effect of a granular system at macro-scale is often studied using the conventional experimental devices and techniques in the laboratories. For example, Jansma (1988) reported that sample size has effect on the macro behavior and indicated that small size samples gain higher strength than large size samples. Hu et al. (2011) indicated that pre-peak behavior is not affected by the specimen size, whereas post-peak behavior depends on the test conditions that control the development of strain localizations. Such conventional experimental devices can merely explore the micro-scale information. Advanced experimental techniques such as the photo imaging analysis (Oda and Konishi, 1974), X-ray tomography (Lee et al., 1992), wave velocity measurement (Santamarina and Cascante, 1996), magnetic resonance imaging (Ng and Wang, 2001) etc. can be used; however, they are complicated, expensive and time consuming. Moreover, not all micro-scale information can be captured using these devices and techniques. It suggests that alternative approaches are required to investigate these micro-scale responses. Numerical approach that models the discrete behaviour of granular materials such as sand can be a good alternative. DEM (Cundall and Struck, 1979) is a numerical tool that draws the attention of many researches to model the discrete behaviour of granular system in recent years. In this study, DEM is used as a numerical tool to study the macro- and micro-scale behavior of granular system for the numerical samples of different sizes. Three numerical samples were randomly generated in three different cubes of different sizes. The randomly generated samples were compressed isotropically by moving their boundaries inward. Simulations of true triaxial compression tests were conducted using these samples to investigate their behaviors at macro- and micro-scale. Digital data at macro- and micro-scale were recorded and the responses were reported.

2. Numerical Method:

DEM is a numerical method that enables one to model the discrete behavior of granular materials. It is pioneered by Cundall and Struck (Cundall and Struck, 1979). The basic idea used in DEM is simple, where each element in the model can make and break contact with its neighbors. Translational and rotational accelerations of particles in a granular assembly are computed using Newton's second law of motion. These accelerations are integrated twice with respect to time to get their displacement. Force displacement law is used to get the forces using the displacement of particles calculated earlier and the cycle continues for the next step. Translational and rotational accelerations of particles are computed as follows:

$$m\ddot{x}_i = \sum F_i \qquad i = 1,3 \qquad (1)$$

$$I\ddot{\theta} = \sum M \qquad (2)$$

where F_i are the force components on each particle, M is the moment, m is the mass, I is the moment of inertia, $\ddot{x}_i$ are the components of translational acceleration and $\ddot{\theta}$ is the rotational acceleration of the particle.

3. Sample Generation And Preparation:

Numerical samples were generated using the open source computer code YADE (Koziki and Donze, 2008) which is based on DEM. YADE is written using C++. Three numerical samples were generated in three cubes of different sizes in such a way that no particle (sphere) can touch others. These generated samples were subjected to isotropic compression by moving their six boundaries inward. The isotropic compression was continued until the unbalanced forces became small and the porosity of the sample at the last few thousand steps became constant. The interparticle friction angles during the isotropic compression for three samples were assigned 0.01° to yield dense samples. The properties of three samples after the end of isometric compression are shown in Table 1. Figure 1(a) shows the initially generated sparse sample S1 whereas Figure 1(b) shows the isotropically compressed dense sample S1 for an example.

Table 1: Properties of three dense samples after the end of isotropic compression

Sample Designation	Size (m×m×m)	No. of Particles	Porosity
S1	0.1×0.1×0.1	2866	0.38
S2	0.125×0.125×0.125	3440	0.38
S3	0.15×0.15×0.15	3897	0.38

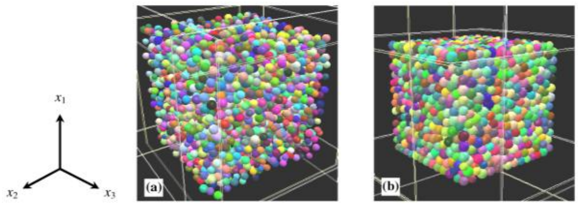

Figure 1: (a) randomly generated sparse sample S1at the initial stage of sample preparation; (b) Sample S1 at the end of isometric compression with reference axes.

4. Numerical Simulation:

Simulation of true triaxial compression test was conducted by slowing moving the top and bottom boundaries inward the sample with a small strain rate and maintaining the confining pressures constant by continuously adjusting the position of other four boundaries of the sample. The isotropically compressed samples of different sizes were subjected to true triaxial compression in drained condition. The DEM parameters used in simulations are given in Table 2.

Table 2: Parameters used in the simulations

Parameters	Value
Box Young Modulus (N/m^2)	60×10^6
Mass density (kg/m^3)	2600
Sphere Young Modulus (N/m^2)	60×10^6
Stiffness ratio	0.50
Strain rate	0.10
Interparticle friction angle (degree)	26.5°

5. Numerical Results:

5.1 Macro-mechanical Responses:

Figure 2 shows the relationship between the deviatoric stress $q\,[=\sigma_1 - \sigma_3]$ and axial strain ε_1, where σ_1 and σ_3 are the stresses in x_1- and x_3-direction, respectively. The deviatoric stress gradually increases with axial strain ε_1 up to peak followed by a huge strain softening. The sample size has no influence on the pre-peak behavior. However, the post-peak behavior is clearly influenced by the sample size. Note that small size sample achieves higher strength than large size sample. This behaviour is consistent with the experimental results (e.g., Jansma, 1988, Hu et al., 2011). The evolution of volumetric strain is also depicted in Figure 3. The volumetric strain is defined here as $\varepsilon_v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$, where ε_1, ε_2 and ε_3 are the strains in x_1-, x_2- and x_3-direction, respectively. The positive value of ε_v indicates compression while the negative value indicates dilation. The samples depict huge dilation after an initial small compression regardless of the sample size which is typical for a dense sample.

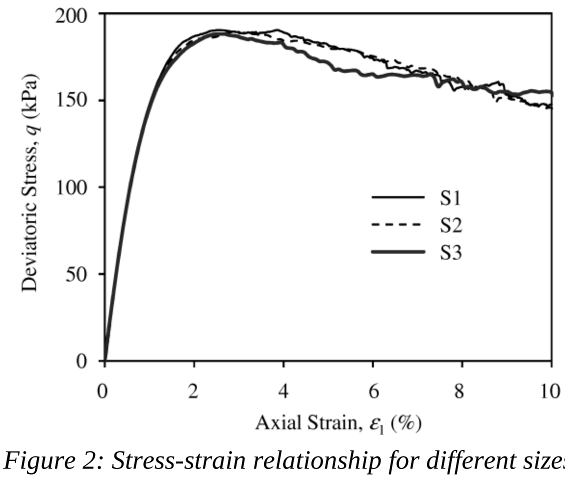

Figure 2: Stress-strain relationship for different sizes of samples

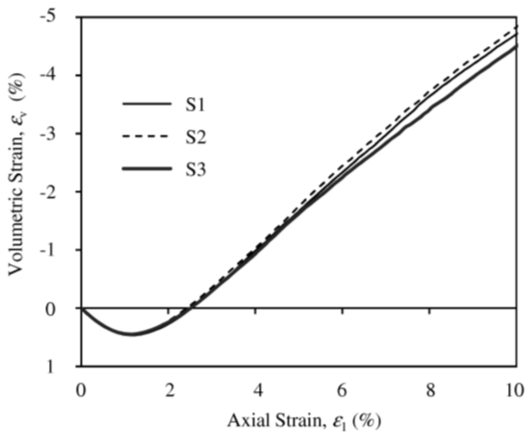

Figure 3: Volumetric strain - axial strain relationship for different sizes of samples

The relationship between the dilatancy index and axial strain is depicted in Figure 4 for samples of different sizes. The dilatancy index is defined here as

$$DI = \frac{-d\varepsilon_v}{d\varepsilon_1} \quad (3)$$

Here, $d\varepsilon_v$ is the change of volume and $d\varepsilon_1$ is the change of axial strain. The dilatancy index curve depicts that the behaviour is almost independent of the sample size. It is also noted that dilatancy index curve becomes almost straight at large strain during the simulation.

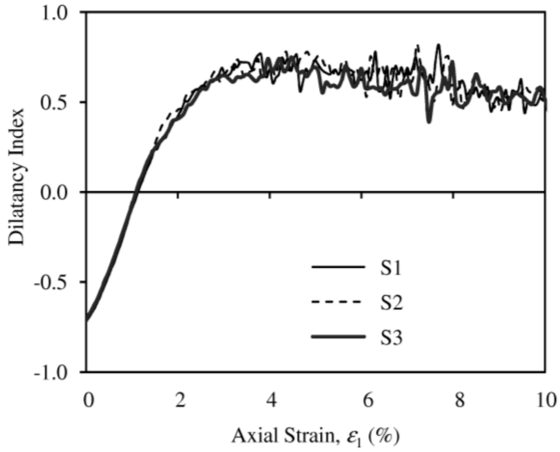

Figure 4: Relationship between dilatancy index and axial strain for samples of different sizes

5.2 Micro-scale Response:

The relationship between the coordination number and axial strain is depicted in Figure 5 for different sample sizes. Coordination number is defined as

$$Z = \frac{2N_c}{N_p} \quad (4)$$

where N_c is the total number of contacts and N_p is the total number of particles. Coordination number gradually decreases with axial strain regardless of the difference in the sizes of samples. The rate of the reduction of coordination number is noteworthy at small strain range; whereas, it decreases for larger strains. Note also that the coordination number is the largest for sample of smallest size.

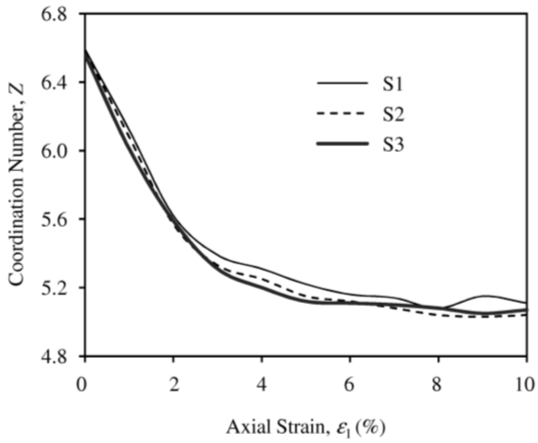

Figure 5: Relationship between coordination number and axial strain for different sample sizes

6. Conclusions:

Numerical simulations were carried out using DEM to investigate the effect of sample size on both the macro- and micro-scale responses of granular materials. Samples of three different sizes were numerically generated and true triaxial tests were simulated. The digital data during the simulation were recorded at regular interval and numerical analysis was conducted. Few important points of the numerical study are summarized below:

- The simulated stress-strain behaviour is qualitatively similar to that observed in the experimental study. This reveals the versatility of the present simulation.
- The dilatancy index behaviour is almost independent of the sample size.
- Coordination number gradually decreases with axial strain regardless of the sizes of the samples.
- Evolution of coordination number is the largest for sample of smallest size.

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