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Simulation of the Behavior of Granular Materials for Varying Void Ratios using DEM

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Abstract: The objective of this paper is to study the behavior of granular materials such as sand under varying void ratios of the samples by two dimensional (2D) discrete element method (DEM) and to quantify the effect of void ratio on different micro-mechanical parameters of granular materials. To achieve the goal, a numerical sample consisting of 8450 ovals was generated in a rectangular frame having a height to width ratio of two without any overlap. The generated sample at this stage was very sparse. Three different samples of different initial void ratios prior to shear were prepared by varying the inter-particle friction coefficient during the isotropic compression stage using the initially generated sparse sample. The initial sparse sample was compressed isotropically to 100 KPa using the periodic boundaries in different stages. The samples were subjected to biaxial shear in strain controlled condition. The simulated data were recorded at required interval and the post analysis was carried out. The simulated macro-mechanical behaviors depict the same qualitative behavior as one observes in laboratory experiments. The work is a function of initial void ratio of the sample prior to shear. However, when the wok is normalized by mean stress, a unique behavior is noticed at smaller strain level regardless of the void ratio of the sample. The evolution of effective coordination number is not much different from that of average coordination number and possesses the same patterns. The evolution of fabric ratio for all contacts does not truly represent the stress-strain behavior, while the evolution of fabric ratio for strong contact represents the stress-strain behavior. A unique correlation between the stress ratio and fabric ratio is observed for small strain level regardless of the void ratio of the sample when the samples are subjected to biaxial shear. However, the same relationship deviates when the strain increases.

Keywords: *Plane Strain Compression, Dilatancy Index, Micro Parameters, Discrete Element Method.*

Introduction:

The physics of granular materials are complex. Sand, gravel, aggregates, powders and rock fill like granular materials are present in nature. Their constitutive behavior is complex because of their inherent granularity. The mechanical behavior of sand and other granular materials depends on the characteristics of its particles. Typically, the granular materials are usually treated as a continuum and their particulate nature is not explicitly considered. An experiment on the theory of voids in granular materials was studied by Worthington (1953). The purpose of this experiment was to study the way in which the void ratio of a granular material depends upon the grading and in particular to find the grading curve which gives the minimum voids ratio. The Voronoi technique was used by Alshibli and El-Saidany (2001) to calculate the local void ratio distribution of granular materials. Xu et al. (2013) have indicated the influence of void ratio on small strain shear modulus of granular materials.

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It was noted that each particle can be applied for a certain soil within a limited void ratio. Small strain shear modulus of granular materials was highly dependent on their current void ratio and stress state.
In the experimental studies, the macro mechanical responses such as stress, strain, volumetric strain, dilatancy index, and so on can be observed easily. By contrast, it is difficult to investigate the micro-mechanical behaviors of granular materials in triaxial and plane strain conditions. It should be noted that the macro mechanical behaviors of any particulate system are the behaviors of the system at the boundaries while the micro mechanical behaviors are the behaviors of any particulate system at the grain-scale level such as the contact geometry between particles, sliding and rolling of each particles, etc. during shear. Nevertheless, the knowledge of the micro characteristics is important to develop physically sound and micro-mechanical based constitutive models. This inherent limitation of experiments can be eluded using the numerical methods such as DEM (Cundall and Strack, 1979), which can provide insights into the micro-mechanical features of granular materials. The evolution of micro-parameters can be inspected and extracted at any stage of simulation. For example, considering the fact, Sazzad et al. (2015) and Sazzad et al. (2016) presented the micro-features of granular materials

under plane strain condition for different void ratios, among others. Even though several studies were conducted by DEM, very few studies were reported in the literature that considered a comprehensive study of macro- and micro-parameters and their inter-relationship for the variations in void ratios. This study presents a comprehensive study of the different macro- and micro-mechanical behaviors of granular materials under varying void ratios of the samples by 2D DEM. For this purpose, four isotropically compressed samples of different void ratios were considered to simulate the behavior of granular materials under varying void ratios of the samples. Isotropically compressed samples having different void ratios were subjected to biaxial compression under strain controlled condition. The macro-mechanical behavior obtained from the numerical experiment was compared with the laboratory experimental results and micro-scale parameters was thoroughly investigated to explore micro-characteristics of granular materials under biaxial compression for varying void ratios of the samples.

Basics of DEM:

DEM has been developed to different levels and applied to a wide range of engineering applications. In a granular medium, forces are transferred only through the inter-particle contacts. The discrete nature makes the constitutive relationship very complex. It was first introduced by Cundall (1971) for rock mass problem and later, extended to soil (Cundall and Strack, 1979). The numerical techniques provide an excellent means to investigate the behavior of granular materials (Vinod et al., 2013). The Discrete Element Method (DEM), also known as the distinct element method, is a multi-scale approach using simple interaction laws for spherical particles whose movements are governed by the fundamental principle of dynamics. In DEM, it is assumed that a material can be characterized by an assembly of rigid particles interacting with one another. The time step chosen should be so small that the disturbance cannot propagate to its immediate neighbors during a single time step. Nevertheless, it is important to note that realistic particle shapes and arrangements are difficult to create and calibrate in DEM. Moreover, relative density is difficult to surmise.

The DEM procedure for contact force calculations and updating the dynamic situations of particles are recognizing the formation of contact point, application of force displacement law, calculation of moment of contact forces and application of Newton's second law of motion. Calculation cycle of DEM involves application of Newton's second law of motion which is given by the following equations:

$$m\ddot{x}_i = \Sigma f_i \qquad i = 1-2 \tag{1}$$

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

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

Computer Program Used:

OVAL (Kuhn, 2006) is a computer program used to simulate the discrete behavior of granular materials in this study. The effectiveness of OVAL has already been recognized (Kuhn, 1999; Sazzad and Suzuki, 2013, Sazzad, 2014). In OVAL, a simple contact force mechanism is included in the system consisting of linear springs in normal and tangential directions and a frictional slider. The coefficients of viscosity for translational and rotational body damping are used in this program that represent a fraction of the critical damping $2\sqrt{mk_n}$ and $2r\sqrt{Ik_t}$, where r , k_n and k_t denote the radius, normal and tangential contact stiffness of the particle, respectively.

Sample Preparation:

Numerical simulation can be divided into two phases: sample generation and sample preparation. At first, a frame was taken with height to width ratio of two. Then, the frame was divided into equal grid. Oval particles were placed on the equally spaced grid points of the rectangular frame such that the center of the grid point and the center of the particle coincide each other. The size of the soil particles and the angle of their position in the grid were chosen randomly. The initial sample generated in the generation phase was very sparse. The initial sparse sample was compressed isotropically to 100 kPa using periodic boundaries in different stages. The sample is compressed to 100 kPa because this confining pressure represents the lateral confinement of a soil element located at a reasonable depth below the ground surface. In the sample consolidation phase, the initial sparse sample was consolidated by assigning interparticle friction coefficient of 0, 0.1. 0.2 and 0.4 for the first, second, third and fourth sample. Then, the rectangular shaped sample was compressed isotropically to 100 kPa using the periodic boundaries. However, the desired interparticle friction coefficient (i.e., 0.5) was used during shear. The void ratios of four isotropically compressed samples after the end of the consolidation are 0.126, 0.164, 0.194 and 0.226, respectively, while the average coordination number of four isotropically compressed samples after the end of the consolidation are 5.5, 4.9, 4.4 and 3.8, respectively. The average coordination number is defined by equation (3).

Simulation of Biaxial Compression Tests:

Simulation of biaxial compression test was carried out by applying a very small strain increment of 0.00002% vertically downward in x_1-direction (parallel to y-axis) and keeping the strain in x_2-direction (parallel to x-axis) constant (100 kPa). The DEM parameters used in the study during shear are shown in Table 1.

Table-1 DEM parameters used in the study

DEM parameters	Values
Normal contact stiffness (N/m)	1×10^{8}
Tangential contact stiffness (N/m)	1×10^{8}
Mass density (Kg/m^3)	2650
Increment of time step (s)	1×10^{-6}
Interparticle friction coefficient	0.50
Coefficient of viscosity for translational and rotational body damping	0.05

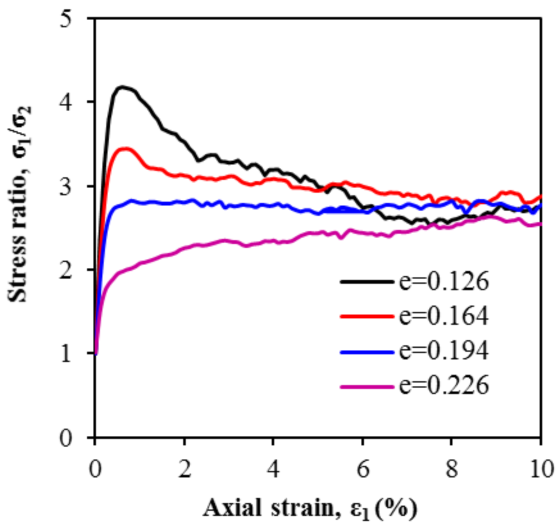

Figure-1 Relationship between stress ratio σ_1/σ_2 and axial strain ε_1

Macro-mechanical Results:

The simulated stress-strain behavior for biaxial compression under different void ratios is depicted in Figure 1. Note that the stress ratio, σ_1/σ_2, for the densest sample (void ratio 0.126) attains a peak at small strain level followed by huge strain softening, whereas for loosest sample (void ratio 0.226), σ_1/σ_2 gradually increases with axial strain ε_1, where σ_1 and σ_2 are the stresses in x_1- and x_2-direction, respectively.

Note also that the stress ratios σ_1/σ_2 for samples having different void ratios come closer at an axial strain of 10 percent, regardless of the void ratio of the samples. This numerical result is consistent with the experimental results under plane strain condition (e.g., Cornforth, 1964).

Figure 2, depicts the relationship between the volumetric strain ε_v and axial strain ε_1. The volumetric strain is defined here as $\varepsilon_v = \varepsilon_1 + \varepsilon_2$, where ε_1 and ε_2 are the strains in x_1- and x_2-direction, respectively. A positive value ε_v in Figure 2 represents compression while a negative value of ε_v represents dilation. Note that the volumetric strain depicts huge dilation in case of the densest sample (void ratio 0.126), whereas the loosest sample (void ratio 0.226) depicts compression. The dilation in dense sample is related to the overriding of the particles due to sliding and rotation in a dense space among the particles. In case of loose sample, particles get more space to move without overriding during sliding and rotation and thus get compressed. Similar tendency as observed in the simulation is noticed in experiments under plane strain condition (e.g., Cornforth, 1964).

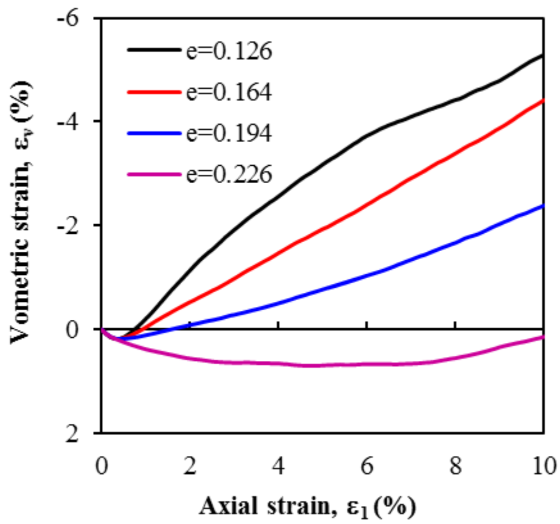

Figure-2 Relationship between volumetric strain ε_v and axial strain ε_1

The relationship between deviator stress $q = \sigma_1 - \sigma_2$ and mean effective stress $p' = (\sigma_1 + \sigma_2)/2$ is depicted in Figure 3. It is noted that deviator stress increases with the increase of mean effective stress. For dense sample, deviator stress is more than loose sample. It is also noted that deviator stress for different void ratio follows a unique behavior. The evolution of the void ratio and effective void ratio is depicted in Figures 4 and 5, respectively. For explanation of effective void ratio, readers are refer to Kuhn (1999) and Kuhn (2006). Note that the evolution pattern of void ratio and effective void ratio is similar. Even though the stress ratio appears to reach almost a critical state; however, the void ratio depicts that the critical state is not yet reached.

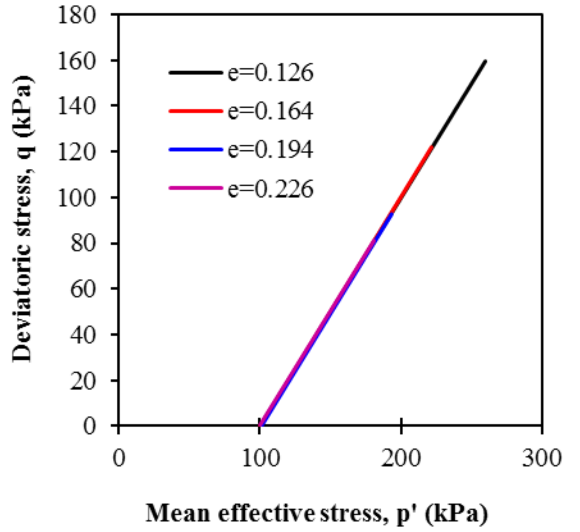

Figure-3 Relationship between deviator stress q and mean effective stress p'

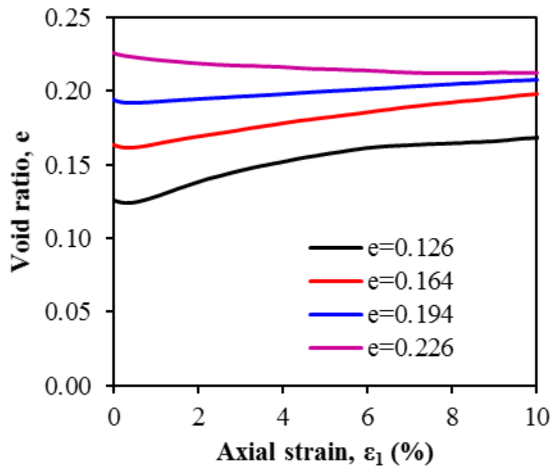

Figure-4 Evolution of void ratio with axial strain ε_1

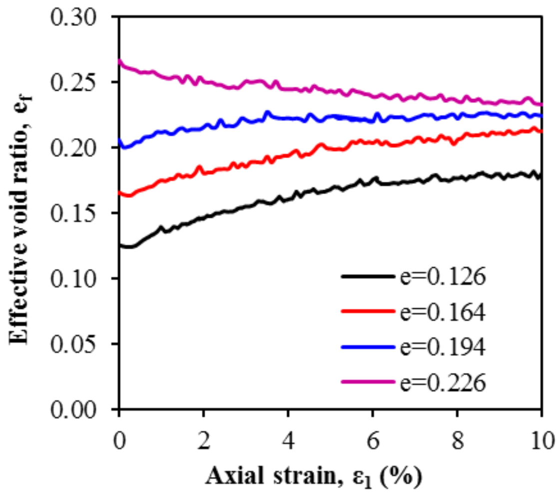

Figure-5 Evolution of effective void ratio with axial strain ε_1

The relationship between work and axial strain is depicted in Figure 6 while the normalized work done for different samples having different void ratios is depicted in Figure 7. The work is normalized by the mean effective stress p'. The work W by the boundary stresses per unit of the original volume of sample is calculated. It is calculated from the work rate $\frac{V_c}{V_i}\int \sigma_{ij}\dot{F}_{ik}F_{kj}dt$ (Kuhn, 2006), where V_c is the current volume, V_i is the initial volume and σ_{ij} is the Cauchy stress and is cumulative from the beginning of the simulation, F is the deformation gradient tensor and dt is the increment of time step. As noticed in Figure 6 that the work is a function of initial void ratio of the sample prior to shear. However, when the wok is normalized by mean stress, a unique behavior is noticed at smaller strain level regardless of the void ratio of the sample.

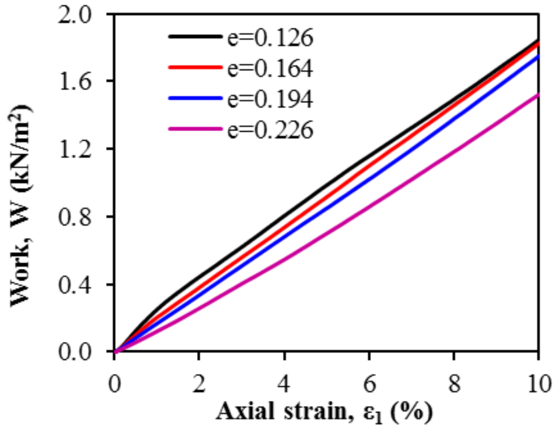

Figure-6 Relationship between work W and axial strain ε_1

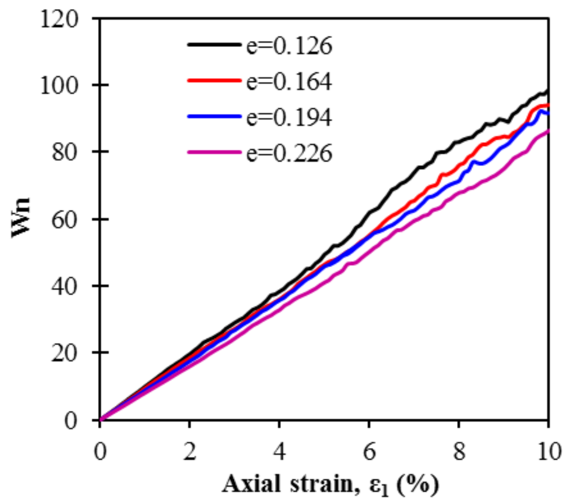

Figure-7 Relationship between normalized work W_n and axial strain ε_1

Micro-mechanical Results:

Figure 8 depicts the evolution of average coordination number with ε_1 while Figure 9 depicts the evolution of the effective coordination number with ε_1 in biaxial compression tests for samples having different void ratios. The average coordination number and effective coordination number are defined as follows (Sazzad, 2014):

$$Z_m = \frac{2 \times N_c}{N_p} \quad (3)$$

$$Z_{eff} = \frac{2 \times \overline{N}_c}{\overline{N}_p} \quad (4)$$

Here, N_c is the total number of contact between particles, N_p is the total number of particles used in the simulation, $\overline{N}_c$ is the total number of effective contact and $\overline{N}_p$ is the total number of effective particles. Contacts are considered to be effective contacts if the minimum number of contacts on a 2D particle are two and the particles involve in effective contacts are considered to be effective particles. For details of effective contacts and effective particles, readers are referred to Kuhn (1999). Note that average coordination number decreases significantly at the beginning of the shear for sample having void ratio of 0.126, which is due to the rearrangement of fabric at the beginning of shear. By contrast, contact disintegration is comparatively lower for sample having void ratio of 0.226. Note, however, that the average coordination number merges each other at larger axial strain indicating almost the same number of contact formation and contact disintegration even though the void ratios are different. Note also that the evolution of effective coordination number is not much different from that of average coordination number and possesses the same patterns.

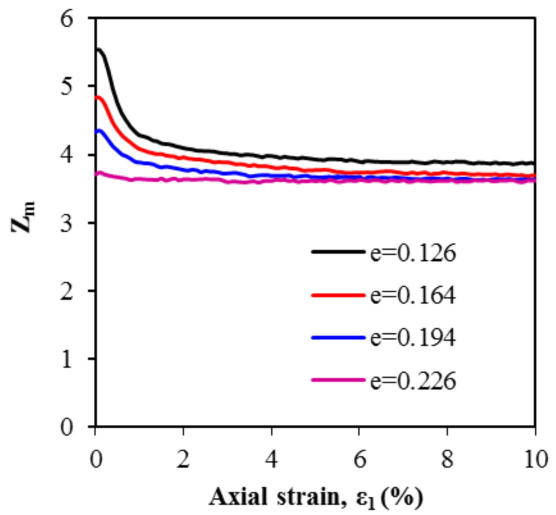

Figure-8 Evolution of average coordination number Z_m with axial strain ε_1

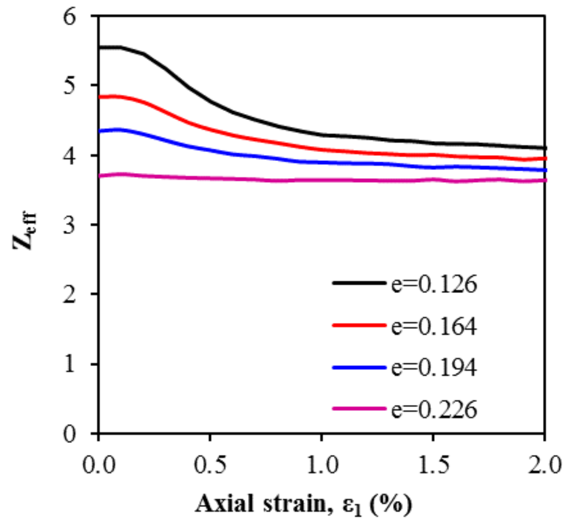

Figure-9 Evolution of effective coordination number Z_{eff} with axial strain ε_1

Figure 10 depicts the evolution of slip coordination number with ε_1. The slip coordination number is defined as follows (Sazzad, 2014):

$$Z_{sl} = \frac{2 \times N_s}{N_p} \quad (5)$$

Here, N_s is the total number of slip contact between particles. Note that slip coordination number peaks at a very small strain level for the densest sample (e=0.126) while peak is not so sharp when the sample becomes loose (e=0.226). It should be noted that slip coordination number merges each other at a moderate level of strain.

The evolution of contact fabric ratio H_{11}/H_{22} for all contact is depicted in Figure 11 while the evolution of contact fabric ratio H_{11}^s/H_{22}^s for strong contact is depicted in Figure 12. The contact fabric for all and strong contact is quantified using the following fabric tensors (Sazzad and Suzuki, 2012):

$$H_{ij} = \frac{1}{N_c} \sum_{c=1}^{N_c} n_i^c n_j^c \quad (6)$$

$$H_{ij}^s = \frac{1}{N_c} \sum_{s=1}^{N_c^s} n_i^s n_j^s \quad (7)$$

where, n_i^c and n_i^s is the components of unit normal vector at c-th contact and s-th strong contact, respectively.

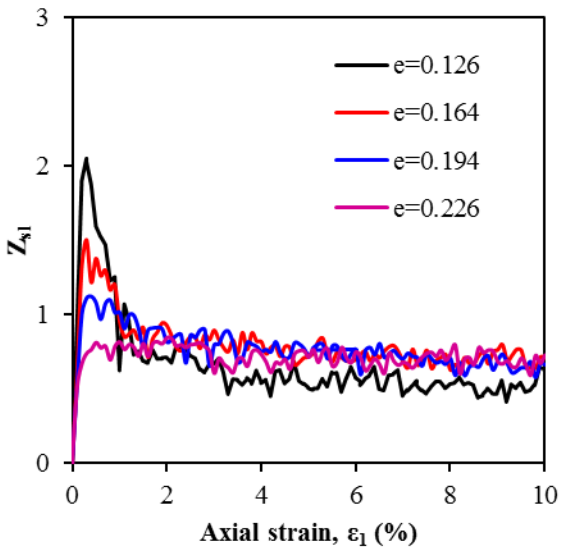

Figure-10 Evolution of slip coordination number with axial strain ε_1

A contact is said to be a strong contact if it carries a force greater than the average force. The average force is calculated as follows:

$$f_{ave} = \sqrt{\frac{\sum_{k=1}^{N_c} \left| f^k \right|^2}{N_c}} \qquad (8)$$

where f^k is the $k-$th force. The evolution of fabric ratios H_{11}/H_{22} for all contact does not truly represent the stress-strain behavior (see Figure 11), while the evolution of fabric ratios for strong contact represents the stress-strain behavior vibrantly. This suggests a linkage between the stress ratio σ_1/σ_2 and fabric ratio H^s_{11}/H^s_{22}.

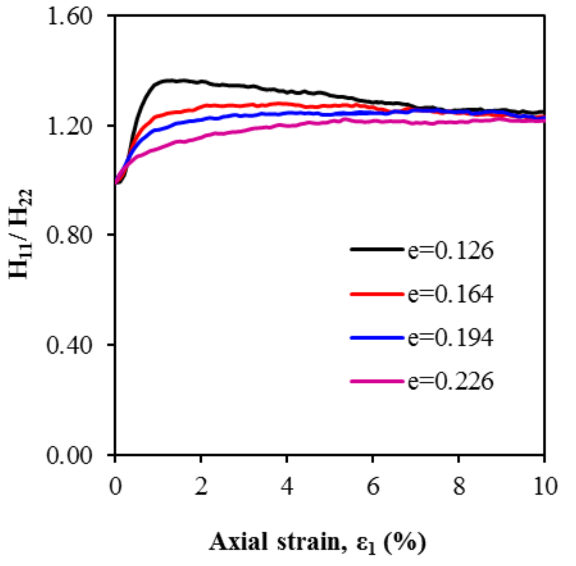

Figure-11 Evolution of fabric ratio with axial strain ε_1 *considering all contacts*

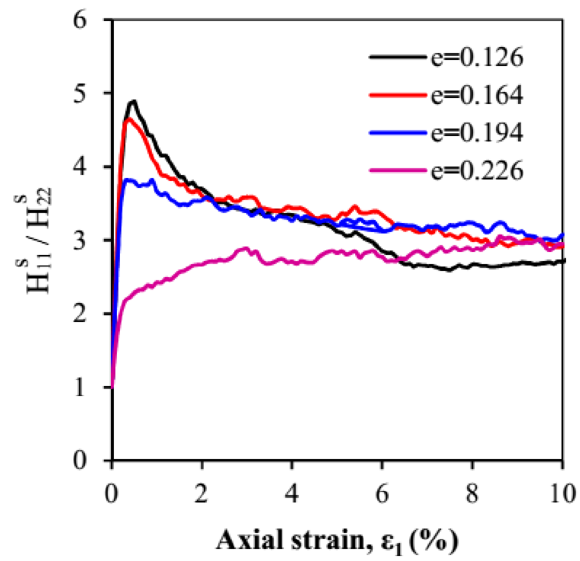

Figure-12 Evolution of fabric ratio with axial strain ε_1 *considering strong contacts*

The relationships between the stress ratio σ_1/σ_2 and the fabric ratio H^s_{11}/H^s_{22} is depicted in Figure 13. Note that a unique correlation between the stress ratio and fabric ratio considering strong contacts is observed at a small strain level regardless of the void ratio of the sample when the samples are subjected to biaxial shear. However, the relationship deviates when the strain keeps increasing.

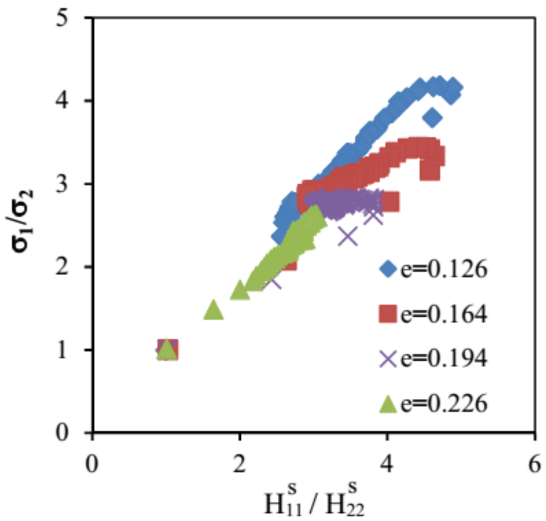

Figure-13 Relation between stress ratio and fabric ratio considering strong contacts

Conclusions:

A numerical simulation is carried out for samples of different void ratios under biaxial compression test to investigate the behaviours of granular materials at micro- and macro-scale level. The simulated behaviours are compared with the experiments qualitatively to warrant the validity of the present simulations. It is observed that the simulated macro results are consistent to that usually observed in experiments. Interesting results related to micro-mechanical behavior are also reported. The evolution of micro-quantities is severely influenced by the initial void ratio of the sample prior to shear. Some of the findings of this study can be summarized as follows:

i) The work is a function of initial void ratio of the sample prior to shear. However, when the wok is normalized by mean effective stress, a unique behavior is noticed at smaller strain level (smaller than 1 percent of axial strain) regardless of the void ratio of the sample. At large strain (larger than 1 percent of axial strain), the normalized work is also a function of void ratios of the samples.

ii) The evolution of effective coordination number is not much different from that of average coordination number and possesses the same pattern.

iii) The evolution of fabric ratio for all contact does not truly represent the stress-strain behavior, while the evolution of fabric ratio for strong contact represents the stress-strain behavior brilliantly. This suggests a linkage between the stress ratio and fabric ratio.

iv) A unique correlation between the stress ratio and fabric ratio is observed at a small strain level regardless of the void ratio of the sample during biaxial shear. However, the relationship diverges when the strain increases (after peak stress).

It should be noted that these conclusions are based on the qualitative comparison of the simulated data with the experiment and further research is necessary to come to a concrete conclusion through a quantitative comparison of simulated results.

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