Abstract

This study presents the macro- and micro-mechanical responses of a sheared granular system using the three-dimensional (3D) discrete element method (DEM). Spheres of different sizes were first generated in a cubic frame in such a way that they were not in contact with their neighbors. This sparse sample was compressed isotropically with a constant confining pressure of 100 kPa. The isotropically compressed sample was subjected to shear deformation with a small strain rate under strain controlled condition. The numerical data were recorded at regular interval to carry out the macro-micro analysis. The numerical result depicts that the simulated stress-strain-dilative responses are in good agreement with the experimental result in a qualitative sense. Different micro parameters were monitored and recorded as well during the numerical simulation. The evolution of these micro-parameters is reported.

Keywords: Granular Materials, Micro-parameter, DEM.

1. Introduction

Granular materials are discrete in nature and their mechanical behavior is complex. Still today, there remain many experimentally observed phenomena that are not clarified and well understood. Specifically, the internal processes that take place during the laboratory experiments are not well known. This is because; these internal processes can not be explored using the traditional experimental devices. Advanced experimental techniques such as the photo imaging analysis [1], X-ray tomography [2], wave velocity measurement [3], magnetic resonance imaging [4] etc. can be employed to understand the internal processes and extract the micro-mechanical data. However, they are sophisticated, expensive and time consuming. Besides, it is not possible to extract all the internal (i.e., micro level) data using these advanced experimental devices or methods. The understanding of these micro-processes is important to develop physically sound models. These micro data is also necessary to explain the physically observed phenomena from the micro-mechanical point of view. The above fact suggests that a comprehensive study is necessary to understand the micro-mechanical characteristics of a granular system. Since it is difficult to conduct experimental study using the conventional experimental facilities, the only alternative is the numerical approach that can model the discrete nature of a granular system. Discrete element method (DEM), pioneered by Cundall and Strack [5], is a numerical method that enables one to model the discrete nature of the granular media. Indeed, the micro-mechanical characteristics have been studied using DEM [e.g., 6-10]; it is still not sufficient and requires further study. In the current paper, the micro-mechanical characteristics of a sheared granular system have been studied in details using 3D DEM. For this purpose, a cubic sample consisting of spheres was generated and compressed isotropically. The isotropically compressed dense sample was subjected to shear under the strain controlled conditions. The digital macro- and micro-mechanical data were recorded at regular interval and their evolution were reported.

2. Numerical method and computer program
The current simulation was carried out using the DEM. The basic idea used in DEM is simple. Each particle in DEM is considered as an element. Each element can make and break contact with its neighbor. The particles can translate and rotate. Newton’s second law of motion is employed to obtain the acceleration of the particle. This acceleration is integrated over time twice to get the displacement. Then the force displacement law is used to get the force using the displacement of the particle calculated earlier. Thus the cycle continues for the next step. For details of DEM, readers are referred to Cundall and Strack [5]. Both the translational and rotational accelerations of the particles are computed as follows:

\[
\begin{align*}
 m\ddot{x}_i &= \sum_i F_i \quad i = 1, 3 \\
 I\ddot{\theta} &= \sum M
\end{align*}
\]

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.

The DEM has been incorporated in the computer code YADE and it has been used to conduct the numerical simulation. The code is written in C++ with Object Oriented Programming and consists of software, libraries and necessary plug-ins. In YADE, one can add new numerical models by only plugging in the corresponding formulas. 3D models of spherical shape particles can be simulated using YADE. It runs on Linux platform. One of the important points in YADE is that it has graphical user interface which allows one to monitor the simulation process during the program run. For details of YADE, readers are referred to Kozicki and Donze [11].

3. Sample preparation

A sparse sample was first generated in a cubic frame such that the particles in the cube were not in contact with each other. Spheres were used as particles as it reduces the computational cost. More than 3800 particles were generated randomly in the cube. The sample was then isotropically consolidated by moving the six rigid boundaries inward with all around confining pressure of 100 kPa. The rate of consolidation was chosen in such a way that the unbalanced forces generated during the consolidation remained fairly small. The consolidation continued for several thousand steps until the confining pressures reached 100 kPa and the porosity of the sample became constant for the last few thousand steps. The interparticle friction angle was assigned zero degree at this stage of consolidation to obtain a dense sample. The state of consolidation simulation was saved in the xml-file format. In the next stage, the xml-file was opened and the interparticle friction angle was replaced by 26.5 degree and the file was saved. The saved file was reloaded and the consolidation continued for the next few thousand steps. When the isotropic consolidation completed, a final state of simulation condition was saved for shear deformation. The porosity of the dense sample at the end of isotropic compression was 0.38. The configurations of the isotropically compressed dense samples with reference axes are depicted in Fig. 1.
4. Numerical simulation
Simulation of triaxial compression test was accomplished by moving the top and bottom boundaries inward the sample at a small strain rate of 0.1 while maintaining the confining stresses in other four boundaries 100 kPa. The confining stresses are maintained 100 kPa by continuously adjusting the position of the boundaries. The stresses in three axial directions and the corresponding strains are measured. The DEM parameters used in the simulations are tabulated in Table 1.

<table>
<thead>
<tr>
<th>DEM parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus (MPa)</td>
<td>60</td>
</tr>
<tr>
<td>Stiffness ratio (Ks/Kn)</td>
<td>0.50</td>
</tr>
<tr>
<td>Mass density (Kg/m³)</td>
<td>2600</td>
</tr>
<tr>
<td>Inter particle friction angles (degree)</td>
<td>26.50</td>
</tr>
<tr>
<td>Damping coefficients</td>
<td>0.20</td>
</tr>
</tbody>
</table>

5. Stress-strain-dilative response
Fig. 2 depicts the stress-strain response of the sheared granular system in strain controlled simulation condition under triaxial compression test for a dense sample. Note that the deviatoric stress $q = \sigma_1 - \sigma_3$ increases with axial strain $\varepsilon_1$ till the peak and then decreases until it reaches the residual state. Here $\sigma_1$ and $\sigma_3$ represent the stresses in $x_1$- and $x_3$- direction, respectively. This tendency is consistent with the laboratory based experimental studies [e.g., 12] in a qualitative sense. This also demonstrates the versatility of the current simulation using the DEM. The evolution of volumetric strain $\varepsilon_v$ with axial strain $\varepsilon_1$ is shown in Fig. 3. Volumetric strain is defined here as $\varepsilon_v = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$, where $\varepsilon_1$, $\varepsilon_2$ and $\varepsilon_3$ are the strains in $x_1$-, $x_2$- and $x_3$- direction, respectively. In Fig. 3, a positive value of $\varepsilon_v$ represents compression while a negative value represents dilation. Note that dilation is the dominant characteristic during the shearing of a dense granular system. This tendency is also qualitatively consistent with the laboratory based experimental studies [e.g., 12]. The evolution of the dilatancy index $DI$ defined here as $DI = -d\varepsilon_v/d\varepsilon_1$ is depicted in Fig. 4.
Fig. 2  Stress-strain relationship for a dense granular assembly sheared under strain controlled simulation conditions

Fig. 3  Evolution of volumetric strain with axial strain for a dense granular assembly sheared under strain controlled simulation conditions
6. Evolution of micro parameter

In this section, the evolution of different micro parameters is discussed. The evolution of the average velocity at any given strain normalized by the average velocity at the end of the isotropic consolidation of the dense sample, $V_t/a/V_{iso}$, with axial strain is depicted in Fig. 5. Here, $V_t/a$ is the magnitude of the average translational velocity at any given strain and $V_{iso}$ is the magnitude of the average translational velocity at the end of the isotropic consolidation of the dense sample. The average velocity is measured from 1% to 10% of axial strain. It is noted that the normalized average velocity has a scattered tendency. Although $V_t/a/V_{iso}$ has a scattered behavior, the maximum value of $V_t/a/V_{iso}$ is observed at 4% axial strain which is close to the peak stress state.
Fig. 6 depicts the relationship between the number of contacts (that carry forces) per particle. It is noted that the contact number per particle sharply decreases at the beginning stage of simulation and later, it becomes almost steady. The loss of contact is due to the dilation of the sheared sample. During dilation, the lateral four boundaries move outward the sample and consequently contact loss takes place.

![Graph showing the relationship between contact number per particle and axial strain](image)

**Fig. 6** Relationship between the contact number per particle with axial strain for a dense granular assembly

### 7. Conclusions

The numerical experiment was conducted under strain controlled simulation condition. Conventional Triaxial Compression (CTC) test was simulated using the DEM. A cubic dense sample consisting of spheres was sheared and the macro and micro-mechanical behaviors were observed. The stress-strain-dilative responses have nice agreement with the experimental tendencies. This reveals the versatility of the current simulation using DEM. The micro-mechanical responses were studies as well. It is noted that the normalized average velocity of the dense assemble is maximum near the peak stress state. It is also noted that the contact number per particle sharply decreases at the begging state of the simulation and later this decrease rate reduces as the strain increase for a dense sample.

### 8. References


