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Simulation of granular material behaviour using DEM

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Abstract

The mechanical response of cohesionless granular materials under monotonic loading has been investigated using a three-dimensional numerical simulation of a standard plane-strain compression test. This paper studies the influence of micro-properties of granular material on the macroscopic stress-strain behaviour observed in the numerical simulation with the discrete element method (DEM). The numerical simulation results are compared with laboratory test on Toyoura sand using model particles of different shapes and sizes with a similar relative particle size distribution. The simulations show that particle properties have a great effect on the soil stress-strain behaviour. The shear strength and friction angle of the sample increase when the particle friction coefficient increases. As the particles become less rotund, the sample shows higher shear strength due to interlocking.

Keywords: discrete element method; plane-strain compression test; granular material; particle shape

1. Introduction

Granular media such as sand composed of discrete particles exhibit very complex macroscopic mechanical responses to externally applied loading. This paper presents an alternative view of granular materials using the discrete element method to investigate their mechanical behaviour at the microscopic level. The discrete element method was first developed by Cundall (1971) for rock mechanics and then applied to granular materials by Cundall and Strack (1979). The first DEM models usually considered the granular materials as assemblies of interacting spheres and reproduced results qualitatively well. However, materials consisting of non-spherical particles behave significantly differently from those consisting of spherical particles (Lin and Ng, 1997). More recent DEM developments focus on the shape of the particle to get more reliable results.

A series of plane-strain compression tests were conducted, with varying initial porosities and confining pressures. The simulated mechanical behaviour of granular materials is compared with those observed from the laboratory tests. The code PFC^{3D} (particle flow code in 3 dimensions) is used. The micro properties of the particles generated in PFC are adjusted to make the macroscopic behaviour similar to that of the real sand. The particles have been simulated using both spheres and clumps (assembly of overlapping spheres struck together). The particle shape effect on the macroscopic behaviour can be studied by comparing the results from the simulations using spheres and clumps respectively.

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DEM provides the possibility to investigate the mechanical behaviour of granular materials at both micro and macro level. The particles used for the simulation follow the relative particle size distribution of Toyoura sand, but proportionally larger. The sand tested in laboratory by Tatsuoka et al (1986) and the results are used for comparison. The simulated sample dimensions were chosen to be the same as for the lab sample (105mm*40mm*80mm), except for the dimention in the plane direction (ie 105mm*40mm*20mm). The specified number of particles can be adjusted by changing the actual particle sizes in proportion to the laboratory particle grading (Figure 1). It reduces the number of particles in the simulation and the calculation time. The actual particle size range in the simulation is adjusted so that the specified number of particles fills the standard sample box at the chosen porosity.

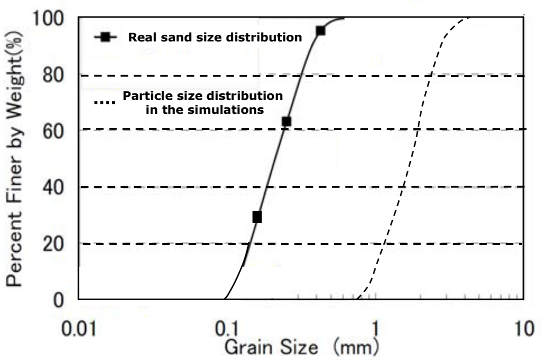

Fig. 1. Particle size distribution of numerical sample and real sand (Builes et al, 2008)

2. Modelling procedure

PFC^{3D} models stressed assemblies by the movement and interaction of rigid spherical particles based on DEM. The model is composed of distinct spheres that displace independently of one another and interact only at contacts or interfaces between the particles. The contact force vector F_i can be resolved into normal and shear components (F_i^n and F_i^s) with respect to the contact plane as

$$F_i = F_i^n + F_i^s \tag{1}$$

The normal contact force is calculated by

$$F_i^n = K^n U^n n_i \tag{2}$$

where K^n is normal stiffness [force/displacement], at the contact and U^n is the overlap of the two entities. The shear force-increment is calculated by

$$\Delta F_i^s = -k^s \Delta U_i^s \tag{3}$$

The new shear contact force is calculated by summing the shear force vector existing at the start of the timestep with the shear force-increment

$$F_j^s = \{F_j^s\}^{[old]} + \Delta F_i^s \tag{4}$$

Where k^s is the shear stiffness [force/displacement] at the contact and ΔU_i^s is the shear component of the contact displacement-increment vector calculated from the motion. In these simulations, the normal stiffness, shear stiffness were chosen as

$$K^n = k^s = k = 1e9 \tag{5}$$

The specific gravity is 2.65.

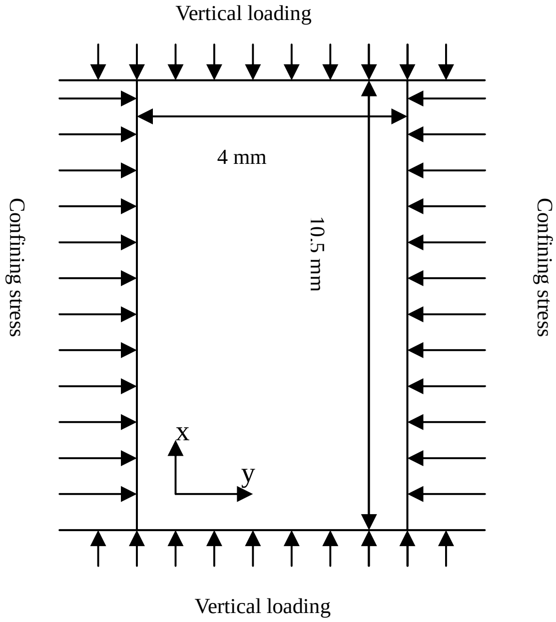

Fig. 2. Schematic illustration of the biaxial test

PFC^{3D} was used to simulate the plane-strain compression test on samples consisting of sphere or clump particles. A cuboidal sample was generated and loaded by the top and bottom walls. The right and left walls were used to maintain the constant confining pressure. The velocities of the top and bottom walls were specified to simulate the strain controlled loading, the velocities of right and left walls were automatically controlled by servo-mechanism to keep the constant confining pressure (Figure 2). The position of the walls was recorded as well as the movement and the contact forces for each particle during the whole simulation for subsequent analysis. The properties of all these walls are assumed to be same. The wall friction coefficient is 0 and wall normal stiffness and shear stiffness are chosen to be the same as particle stiffness, 1e9 N/m.

2.1. The parameters chosen for simulations

The sample consists of spheres particles or clump particles. The maximum particle radius for each sample was 2.05mm and the minimum radius was 0.5mm, which was about 10 times the size of the real sand (Figure 1). Figure 3 shows model particles of single spheres or two-ball clumps. A clump is an agglomerate of overlapping spheres. Each clump here comprises two sphere particles of different sizes. R and r are the radii of the larger and smaller spheres respectively. L is the distance between the centres of two spheres in each clump. The relationships among them are L=1.5R and R=0.75r. The clumps were formed by creating initial spheres, of the same size as the simulations using spherical particles (the dashed line in Figure 3). “Virtual spheres” were then created by deleting the initial spheres and creating a virtual space by multiplying the initial sphere diameter by a factor of 1.31. Each “virtual sphere” formed the outermost possible boundary for each clump and the clumps were created with the “virtual spheres”. For the clumps, the stiffnesses and coefficients of friction used were the same as for the simulation of spheres. The void ratios for these samples are all 0.70. All the particle parameters are identical. Particle friction coefficient is 0.7 and the normal stiffness and shear stiffness of particles are 1GPa.

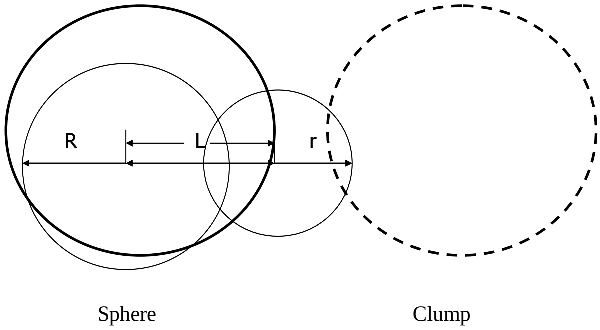

Fig. 3. Particle shapes in the simulations

2.2. Sample generation

Six walls were generated as sample boundaries. Particles were generated to fill into this space. The samples were generated by the particle radius expansion method. This is used to place a specified number of particles at random coordinates within a given space. A population of particles with artificially small radii is created within the specified volume because a new particle will not be placed if it would overlap another particle or a wall. The particles are then expanded until the desired porosity is obtained. The number if particles was required to satisfy the specified particle size distribution (Figure 1), void ratio and sample size. The void ratio defined as:

$$e = \left[bht - \sum_{1}^{N} \frac{4}{3}\pi r_i^3 \right] \Big/ \sum_{1}^{N} \frac{4}{3}\pi r_i^3$$

where b is the wideness of the sample, h is the length of the sample, t is the thickness of the sample. N is the total number of the particles. Figure 4 shows a sample with 15000 spheres and voids ratio of 0.7.

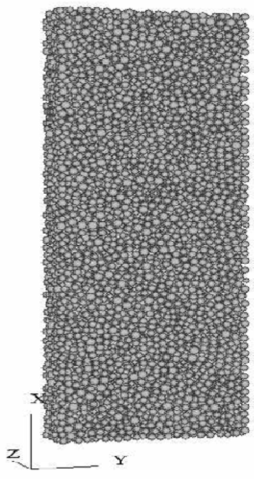

Fig. 4. A sample of spheres

After the sample is generated, the sample stress state is adjusted to $\sigma_x = \sigma_y = \sigma_0$. σ_0 is the initial consolidation confining pressure. σ_x and σ_y are defined as the axial stress and confining stress, calculated from the contact forces and the ball/wall contact areas:

$$\sigma_x = \sum f_x / bt$$

$$\sigma_y = \sum f_y / ht$$

where $\sum f_y$ is the resulting contact force acting on the right and left walls and particles; $\sum f_x$ is the resulting contact force acting on the top and bottom wall and particles.

The loading was carried out by moving the top and bottom walls at a rate 0.02mm/s after the sample reached the initial state. The initial state is defined such that after one numerical sample has been generated at the required porosity, a confining stress σ_0 of 400kPa is applied to the boundaries and the sample is allowed to come to equilibrium. The loading and the confining pressure are applied on the sample by top, bottom walls and right, left walls. The sample thickness was fixed by front and back walls to simulate the plane-strain condition. For the z direction, the walls were fixed. In each of the tests, the sample has about 15000 particles with spheres or clumps.

3. **Results and discussion**

The purpose of the simulations is to get a similar typical behaviour of sand in comparison with experimental results. In this part, effects of interparticle friction and particle shape will be discussed. For the sample comprising spherical particles, different particle friction coefficients are used in the simulations to investigate the effect of particle friction coefficient. The clump of overlapping bonded spheres is used in the simulations to investigate the effect of particle shape.

3.1. Experimental

Tatsuoka et al (1986) performed a series of drained plane strain compression tests on saturated samples of fine angular to sub-angular sand (Toyoura Sand) at confining pressure 400kPa. The samples were prepared by the air-pluviation method with changing the angle δ of bedding plane to the σ_1'- direction during plane strain compression tests from 0 to 90 degrees.

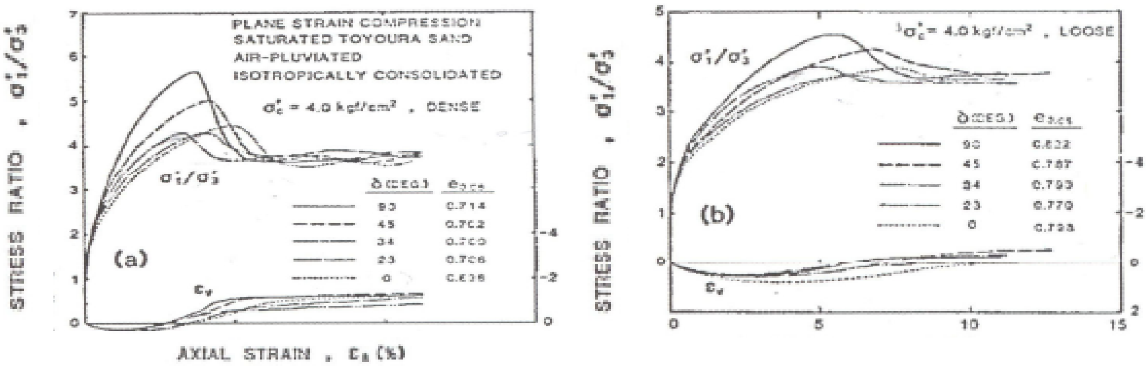

Fig. 5. Typical stress-strain relations for tests at σ_c'=400kPa for both dense and loose samples

The nominal initial sample dimensions are h_0 (height) =10.5cm, w_0 (length in the σ_3'-direction) =4cm and l_0 (length in the σ_2'-direction) =8cm.

The typical relationships between stress ratio, axial strain and volumetric strain they got are shown in Figure 5. These curves describe the results from anisotropic samples with different angle δ from 0 to 90 degrees. The simulation results will be compared with these experimental results.

3.2. Effect of interparticle friction angle

Simulation of a material's macro behaviour using DEM is difficult as the choice of micro-properties is complicated. The particle properties have an important effect on the macro behaviour. The spherical particles are used in these simulations with different particle friction coefficients.

Figure 6 shows the stress-strain relationship with different friction coefficients when the initial voids ratio is 0.70. The strain hardening model is observed when the particle friction coefficient is small. After the peak value, a strain-softening behaviour is observed when the friction coefficient is sufficiently high. The peak of the stress-strain curve increases when the friction coefficient increases. Figure 7 shows that the volumetric dilation increases when the friction coefficient increases. The samples include spherical 15000 particles with a confining stress of 790KPa.

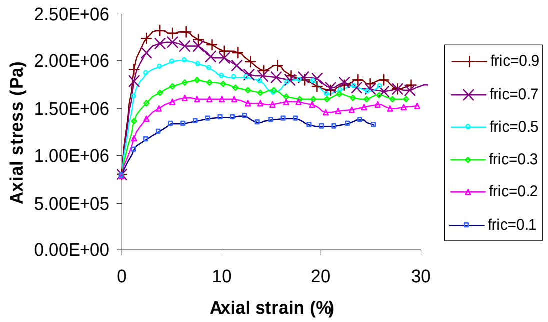

Fig. 6. Stress-strain relationship (using spheres, σ_3 =790kPa)

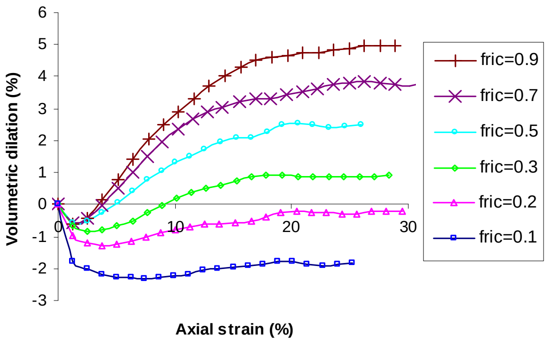

Fig. 7. Volumetric dilation against axial strain (using spheres, σ_3 =790kPa)

The results show that the friction coefficient between the particles has a large effect on the peak of sample strength, as well as the overall sample dilation at the end of shear. These results are consistent with previous studies (Ni, 2003). For comparing with experimental results, three simulations using particle stiffness (1e9), particle friction coefficients (0.5, 0.7, 0.9) and sample void ratio (0.7), confining pressure (400kPa) are performed, the results are shown in Figure 8 and Figure 9. But these samples strength are much lower than the experimental result (Figure 5). So the influence of particle shape on the sample strength will be examined.

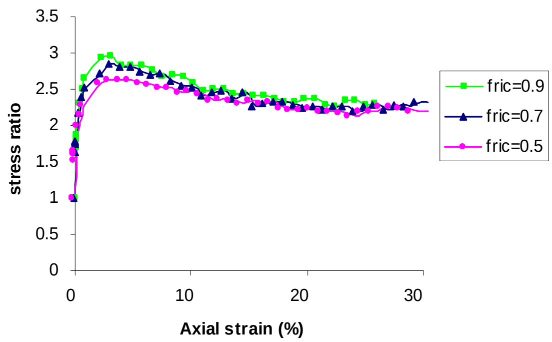

Fig. 8. Stress ratio against axial strain (using spheres, σ_3 =400kPa)

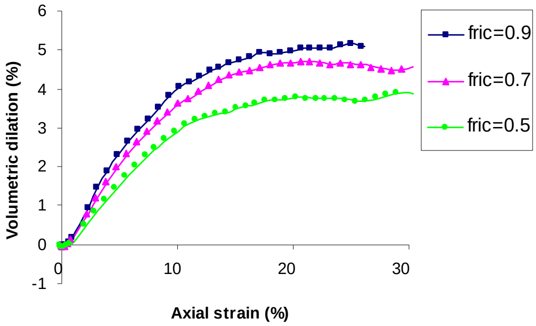

Fig. 9. Volumetric dilation against axial strain (using spheres, σ_3 =400kPa)

3.3. Effect of particle shape

The spherical shape is too idealized to represent real granular material elements like sand grains. The real sand particle is irregular and involves more complex intergranular interactions than between spheres. So clumps were used in the simulation. The shape of clump is shown in Figure 3.

The simulation results by using spherical particles and clumps are compared with the experimental result from Tatsuoka (1986). The samples using in the laboratory test are anisotropic, but the samples using in the simulations are isotropic. So select two results from experimental results (Figure 5), one result with δ=90º (top line in Figure 10) and one result with δ=0º (second line to top in Figure 10). As shown in Figure 10, the bottom line is the simulation result with spherical particles and the simulation result by using clumps is shown as the second line to bottom. The simulation result with spherical particles is selected from Figure 8 with particle friction coefficient 0.7. These two lines from simulations are quite similar at the beginning, and after that the middle line get the peak value higher than bottom line almost at the same axial strain. And then both of these two lines drop down a little. The result using clumps gives larger peak stress ratio and higher ultimate stress ratio.

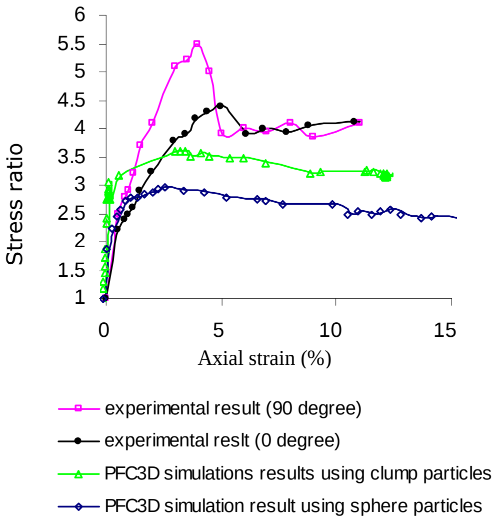

Fig. 10. Comparison between results from PFC^{3D} simulation and experimental data (σ_3 =400Pa)

The material used in the laboratory test is a sub-angular sand (Toyoura sand). The particle shape must be the principal reason to affect the material behaviour in the simulations. Figure 10 shows the effect of particle shape. We can see that the middle line is closer to the top line. That means the simulation with clumps is similar to the laboratory result than the one with spheres. More generally, the particle shape has an important effect on the granular material behaviour. The strength of sample increased significantly when particles became less spherical.

4. Conclusions

In this paper, granular material behaviour is investigated by the numerical approach with the aid of DEM. While the experimental approach works at a macroscopic level, the numerical method has the advantages of providing the mechanical behaviours of the granular assembly at both the macro- and micro- scales. The mechanical response of cohesionless granular material under monotonic loading is studied.

DEM successfully simulates the typical granular material behaviour in the plane-strain compression mode, as observed in experimental tests.

The comparison of the simulation results with the laboratory results shows that the results from clump particles sample are better than the results from samples of spherical particles.

The simulations show that particle properties have a great effect on the soil stress-strain behaviour. In these simulations, both spherical shape and non-spherical shape of particle have been used. They show that particle shape and friction coefficient have a significant effect on the sample strength. The shear strength and friction angle of the sample increases when the particle friction coefficient increases and when the shape is irregular.

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