Particle flow simulation of constitutive behavior of sands

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Abstract. Particle Flow Code, based on the method of discrete element, overcomes the hypothesis of macroscopic continuum in traditional mechanics model, and can simulate the properties of sands with the linear and the hertz-mindlin contact model in microscopic level. Triaxial shear test of sands is simulated by PFC2D biaxial confined test, and then the effects of microscopic parameters, such as the shear modulus, poisson’s ratio, particle radii, particle shape, contact stiffness, etc., and the confining stress on the macroscopic mechanical properties of sands (dilatancy, phase transformation, fabric, etc.) have been discussed. And finally the microscopic parameters of sand have been calibrated for further study by two contact models respectively.

1. Introduction
Conventional particle flow models can be used to simulate the mechanical behavior of a collection of systems of particles of arbitrary shape. The concept of "particles" here is different from the concept of particles in mechanics in the broader sense. The volume of particles is often ignored and the particles that make up this model are independent of each other, and interaction forces occur only at the interface or contact surface.

A PFC2D model is composed of a set of two-dimensional circular particles. The PFC2D program is based on the discrete element method [1][2] and uses a rigid disc or sphere as the basic unit, using the motion and interaction of the basic unit to simulate practical problem which contains the following assumptions [3]: (1) The basic unit is a rigid disc or ball. (2) The contact range between the particles is much smaller than the particle size which is close to the point contact. (3) The contact between the particles is a flexible contact, and a certain overlap is allowed at the contact. (4) The contact force between the particles is related to the amount of overlap of the particles. (5) Different shapes of units can be composed of particles.

The particle discrete element numerical method have been widely applied to the research results of soil mechanics, for example, ZhouJian et al.[4] carried out particle discrete element numerical simulation of soil failure meso-mechanism and piping phenomenon meso-mechanism, meanwhile, ZhouJian et al.[5]adopted PFC2D constant volume cyclic biaxial test conditions to conduct numerical simulation of particle flow for liquefaction of sandy soil under undrained cyclic load, and all the results were basically consistent with the tests. LuoYong et al.[6] used PFC2D / PFC3D software to carry out numerical simulations of the surrounding structures such as pile walls and braces. The results suggest that PFC2D method can be used to analyze the macroscopic mechanical response of the envelope structure under external load. Masson et al.[7] used the PFC2D method to analyze the direct
shear characteristics of two-dimensional particle aggregates, and obtained the typical macroscopic shear behavior of granular materials such as loose sample shrinkage, compact sample dilatation and strain softening, and the formation mechanism of the shear band was also analyzed from the meso-levels of displacement and particle rotation. Chi Yong[8] analyzed the basis of the influence of the changes in the mesoscopic parameters of the contact stiffness model on the macro-mechanical properties of the biaxial specimen, meanwhile, based above, the meso-mechanical mechanism of the formation and development of shear bands in sands and cohesive soils were studied using the PFC2D method, and compared with the laboratory test laws.

Since the particle flow samples are actually based on the microscopic characteristics of the granular medium itself, the interactions between the particles in the PFC2D[3] numerical model reflect the meso-mechanical behavior of the granular medium skeleton, i.e., it is actually the constitutive behavior of the soil skeleton. So this paper below will discuss the macroscopic stress-strain characteristics of the soil medium simulated by the particle flow sample based on the linear contact model and the hertz-mindlin (H-M for short)contact model.

2. Study on particle mechanical parameters of sands for confined biaxial test-linear contact model

Coarse-grained soil (sandy soil) is also called non-cohesive soil, and the particles are in point contact. The granularity and disintegrability of sandy soil are very suitable for simulation with granular aggregates. The confined biaxial test is often used for numerical experiments to study the mechanical properties of sandy soils. At present, there are studies on the confined biaxial test of the mechanical properties of the shear band of sands, loose sands and dense sands under monotonic and cyclic loading [5][6][9].This paper uses the particle mechanics method to study the particle mechanics influencing factors of sand mechanical properties. The particle mechanical parameters include particle density $\rho_{se}$, average particle radius $R$, the ratio of the maximum and minimum particle diameters, the planar porosity of the particle assembly $n$, particle friction coefficient, normal tangent stiffness of particles $k_n$, and shear stiffness $k_s$ (linear contact model) or shear modulus $G$ and poisson's ratio of particles $\nu$ (H-M contact model).

Preparation of numerical sample for sands is to set the size as 0.0945m×0.0377m that is close to the actual conventional triaxial sample size in appearance size. The particle unit is a two-dimensional disc unit[1], the average particle size is 0.001m, and the sample is generated by the radius expansion method and the initial porosity is 0.12, the particles follow a uniform distribution, $R_{max}/R_{min} = 4$, the number of particles generated is 997. The density of the particles is taken as the density of quartz sand 2650kg/m3, The cohesion parameter is zero, the sample is loaded using a strain-control method, the loading rate of the test is constant, the upper and lower walls are relatively moved at a loading rate of 0.4 m/s, and the sample is consolidated using an isotropic consolidation method. The confining pressure is 2Mpa, while the lateral confining pressure is kept constant to simulate the drainage and shear conditions of the indoor test. The numerical sample parameters are shown in table 1 below.

| sample dimension/mm | particle density/kg.m$^{-3}$ | maximum particle size/mm | minimum particle size/mm | initial void ratio | particle number | confining pressure/MPa |
|---------------------|-----------------------------|--------------------------|--------------------------|-------------------|----------------|-----------------------|
| 94.5×37.3           | 2650                        | 0.16                     | 0.04                     | 0.12              | 997            | 2                     |

When loading, the average of the upper and lower wall stress are defined as the major principal stress $\sigma_1$; The average of the left and right wall stresses is the minor principal stress $\sigma_3$; The strain caused by the movement of the upper and lower walls is the major principal strain $\varepsilon_1$; The strain caused by the left and right wall movement is the minor principal strain $\varepsilon_3$; The sum of the major and minor principal strains is the body strain $\varepsilon_s$. Research parameters include: confining pressure, particle
friction coefficient $\mu$, the stiffness of the particles themselves $k_n$, $k_s$ (linear model), $G$, $\nu$ (non-linear model), particle size ratio (non-linear model), the peak strength, strain, and secant modulus of different parameter curves $E_r$ obtained at the 1/2 peak intensity.

The so-called particle flow numerical simulation sample is actually to change the meso-mechanical properties of the particle unit and its aggregate structure, so as to approximate the macro-mechanical response of real materials. Therefore, the numerical simulation of rock and soil samples by particle flow theory is a process of continuously modifying and debugging various meso-mechanical parameters (including particle size). The sample simulation adopts a linear contact model, and the mesoscopic parameters are shown in Table 2.

Table 2. Mesoscopic parameters for sand samples

| Parameter | Value  |
|-----------|--------|
| $k_n$ (Pa) | 9e8    |
| $k_s$ (Pa) | 4e8    |
| $G$ (Pa)   | 40e9   |
| $\mu$      | 0.5    |
| $\nu$      | 0.35   |

Figure 1. Stress/Stress ratio- strain relationship with regard to different confining pressures for sands

Figure 2. Relationship between volume strain and axial strain at different confining pressures
Figure 3. Relationship between phase transformation void ratio and positive stress at different confining pressures [10]

Figure 4. Mean effective stress-void ratio relationship at different confining pressures

Figure 5. Relationship between fabric parameter ($\varphi_1 - \varphi_3$) and deviatoric stress ratio for different confining pressure [11]
The figures above show that the changes between shear stress and axial strain, volumetric strain vs axial strain, fabric vs shear stress ratio, normal stress vs phase transformation porosity ratio at different confining pressures (2Mpa, 4Mpa, 6Mpa, 8Mpa, 10Mpa)[10]. It can be found that as the confining pressure increases:

(1) The peak strength of the "sample" and its corresponding strain increase significantly, and the deformation modulus of the "sample" corresponding to the secant modulus at half the peak strength increases slightly.

(2) The peak stress ratio is getting smaller and smaller, the stress ratio-axial strain curve is getting smoother and the strain softening section is weakening.

(3) When the phase transformation state is reached, the corresponding axial strain gradually increases, the corresponding compression increases, and the subsequent dilatancy trend is the same.

(4) For soil samples with the same initial state, the phase transformation porosity obtained under different confining pressures and their corresponding normal stresses are approximately linear in semi-logarithmic coordinates.

(5) Anisotropic coefficient of sample particle contact normal \((\phi_1-\phi_3)\) [11] (Note: the subscripts 1 and 3 represent the direction of the major stress respectively) gradually decrease. Under the same confining pressure, the particle contact normal anisotropy coefficient \((\phi_1-\phi_3)\) varies linearly with the deviatoric stress ratio.

### 2.1 Consider gravity effects

![Figure 6. Relationship between deviatoric stress ratio and axial strain: no gravity vs gravity](image)

From the consideration of the variation curves of the deviatoric stress ratio-axial strain, phase transformation porosity ratio-normal stress under gravity, it can be found that under the condition that other factors are unchanged, the effect of gravity is considered to make the obtained deviatoric stress ratio relatively high. The reason is that the direction of gravity is the same as the direction of the major principal stress, that is, close to the direction of the strong chain, so the obtained partial stress is higher than the deviatoric stress obtained no gravity exists, and the greater the confining pressure is, the greater the difference in stress when there is no gravity-induced.

From the obtained volumetric strain-axial strain curve, it can be found that when gravity exists, the axial strain corresponding to the position where the phase transformation occurs correspondingly increases, and the compression increases which is equivalent to the mechanical effects caused by the increase in normal stress; From the obtained phase change porosity-normal stress curve, it can be found that on the e-logp plane, the change curve is approximately linear, and the e-logp line under the influence of gravity is located below, but the difference is small; From the obtained curve of contact normal anisotropy coefficient and deviatoric stress ratio, it is found that anisotropy is caused by gravity, and the larger the confining pressure, the greater the impact.
Figure 7. Volumetric strain-axial strain curves at different confining pressure: no gravity vs gravity

Figure 8. Relationship between phase transformation void ratio and positive stress: no gravity vs gravity [10]

Figure 9. Fabric parameter (φ1 - φ3) vs axial strain curves under different confining pressure for sands
2.2 Consider the effects of the coefficient of friction

As shown in Figure 10, from different friction coefficients (μ = 0.3, 0.5, 1.0), the comparison of the stress-strain, volumetric strain-axial strain relationship curves can be found that as other factors are unchanged, the peak value of the stress-strain relationship curve will increase significantly with the increase of the friction coefficient, and the initial elastic modulus will also increase to some extent; The larger the friction coefficient, the more obvious the softening phenomenon, and the smaller the friction coefficient corresponds to the ideal elastoplastic relationship, and the increase of the friction coefficient leads to the obvious softening phenomenon; It is found from the relationship between volume strain and axial strain that the larger the friction coefficient, the more compression, and the dilatancy trend becomes more prominent in the later stage, and the corresponding phase transformation stress ratio increases with the increase of the friction coefficient.

![Figure 10. Effects of frictional parameters on the mechanical behavior of sands](image)

2.3 Effects of particle contact stiffness on stress-strain curve

It can be seen from Fig.11 that the contact stiffness ratio kn/ks has a greater effect on the stress-strain curve of the sandy soil sample. Obviously, as the normal contact stiffness kn increases, the initial elastic modulus of the specimen increases, and the strain corresponding to its peak strength will decrease; The change in the tangential contact stiffness ks has little effect on the initial elastic modulus. Although the sample peak intensity has an effect, it is not large. As can be seen from Fig. (b), as the contact stiffness ratio kn / ks increases, the dilatancy increases significantly, and the stiffness ratio directly affects the change in poisson's ratio. In addition, although the stiffness ratio kn / ks = 9/4 is less than kn / ks = 9/4, but ks is relatively large, so its corresponding peak value and dilatancy are more obvious.
2.4. Effects of particle size ratio on mechanical behavior of sand samples

As shown in Figure 12(a), for sand samples, the effect of the maximum / minimum particle size ratio (as a function of the porosity ratio of the sample) on the peak strength of the stress-strain curve is not large, and the figure (b) shows that the particle size ratio has no effect on the location of the phase transformation of the sand, but it has a larger effect in the later stage of dilatancy.

2.5 Effects of particle shape coefficient on mechanical behavior of sand

PFC2D calls the "clump"[12] command to form two circles "blocks", so the original contour characteristics of the particles are changed, and the circle (F = 1.00) and the oval-like shape (F = 0.91) are selected [12]. As shown in the figure 13, the peak strength increases with the decrease of the shape coefficient, as well as the compression increases, and the later dilatation is obvious. This is interpreted as follows: The more irregular the particle shape, the more obvious the occlusion between particles, the greater the resistance of the particles to overcome that lead to the increase in the strength of the particle group. As the shape coefficient decreases, the softening effect of the material becomes more obvious which may be due to the more irregular the material. During the process, the particles roll and climb more strongly between each other. After the peak stress is exceeded, the stress softening is even more severe.
3. Study on particle mechanical parameters of sand confined biaxial test-H-M contact model

The contact stiffness models provided by PFC2D include linear contact model and H-M nonlinear contact model[3]. Above studies on the effects of mesoscopic parameters are mainly developed for linear contact models. The following will discuss the effects of granular materials on the macro-mechanical response of sands. The mesoscopic parameters of the linear contact model are normal contact stiffness \( k_n \), tangential contact stiffness \( k_s \), and particle friction coefficient \( \mu \) as well as the shape factor \( F \). The effect of the changes in the mesoscopic parameters on the macro-mechanical properties of the sandy soil numerical samples when the linear contact model is used is analyzed in detail above. The research results show that the contact stiffness between particles mainly affects the macroscopic deformation modulus of the sample and the strain when the stress peak appears; The particle friction coefficient mainly controls the magnitude of the peak strength and has a large effect on the dilatancy; The ratio of normal contact stiffness to tangential contact stiffness \( k_n / k_s \) not only affects the peak intensity, and has a greater impact on the volume change, that is, the size of the macro poisson's ratio.

The mesoscopic parameters of H-M contact model include meso-shear modulus \( G \), poisson's ratio \( \nu \) and particle friction coefficient \( \mu \). The following tests will use the biaxial numerical test conditions to analyse the effect of changes in the meso-parameters of the H-M contact model on the macro-mechanical properties of the sand sample.
Preparation of "sample" for sand particles is to set the size as 0.0945m × 0.0377m, average particle size is 0.001m, initial porosity is 0.12, particle arrangement obey uniform distribution, \( R_{\text{max}}/R_{\text{min}} = 4 \), the number of particles generated is 997. The density of the particles is 2650 kg / m³ of the quartz sand, the cohesion is zero, the loading rate of the test is constant, and the confining pressure is controlled at 0.2Mpa.

| Table 3: Mesoscopic parameters for H-M contact model |
|-----------------|-----------|-----------|
| \( G \) (Pa)   | \( \nu \) | \( \mu \) |
| 5e11            | 0.35      | 0.5       |

3.1. Shear modulus \( G \) impact

In order to analyze the impact of mesoscopic shear modulus \( G \), here we fix meso-poisson ratio \( \nu = 0.35 \), particle friction coefficient \( \mu = 0.5 \), then the picture shows the relationship between the partial stress-axial strain and the body strain-axial strain of the sample when shear modulus \( G \) changes in the range of 2e11 ~ 5e11Pa.

As can be seen from Figure 15( a), the effect on the macroscopic deformation modulus of the sample is very significant. The average deformation modulus of the sample corresponding to the secant slope of the stress-strain curve at half of the peak intensity significantly increases, at the same time, the peak intensity also increases to a certain extent, and the failures strain decreases when the peak appears.

As can be seen from Figure (b), it has a great influence on the shear expansion and contraction characteristics of the sample. With the increase of the value \( G \), the volume shear shrinkage deformation of the sample at the initial stage of loading is obviously reduced, and the sample has a dilatancy trend at a small axial strain.

3.2. Particle friction coefficient \( \mu \) impact

To analyze the impact of particle friction coefficient \( \mu \), it is always to fix mesoscopic shear modulus \( G \) and meso-poisson's ratio \( \nu \). The pictures show the macroscopic stress-strain and volume strain-axis strain curves of the sample when \( \mu \) changes within the range \( \mu = 0.2 - 0.6 \).

As can be seen from figure (a), the particle friction coefficient \( \mu \) has a greater effect on the peak intensity of the sample. The increase of the peak intensity is very obvious, and the corresponding axial strain also increases, but the effect on the deformation modulus is not significant. As can be seen from figure (b), it has a small effect on the position when the phase change occurs, but it affects the dilatancy trend of the sample. The larger the value \( \mu \), the more obvious the tendency of the specimen to dilate.
Figure 16. The effect of frictional parameter $\mu$ on the mechanical behavior of sands

3.3 Poisson’s ratio $\nu$ impact

As well, when analyzing the impact of poisson's ratio $\nu$, it is always to fix mesoscopic shear modulus $G=2\times10^{11}$ and particle friction coefficient $\mu=0.5$. Figure 17 show that when the value $\nu$ is within the range of 0.16 ~ 0.5, the stress-strain and volume strain vs axial strain relationship curves of the sample.

As can be seen from the figure 17, with the increase of meso-poisson ratio $\nu$, the macroscopic deformation modulus and peak strength of the sample both increase slightly, but the change isn’t significant. As shown in figure (b), except for the occurrence of dilatancy, the axial strain varies with $\nu$, the increase is slightly reduced, under the conditions, the shape of the volume strain vs axial strain curves is very close. Above analysis results show that with the change of meso-poisson ratio $\nu$, it has little effect on the macro-mechanical response of the sample.

Figure 17. Effects of poisson's ratio $\nu$ on the mechanical behavior of sands

4. Comparison of linear contact model and H-M model

The effects of the mesoscopic parameters for two kinds of models on the macro-mechanical response of numerical specimens are discussed above. When using a linear contact model, the macroscopic deformation modulus of the specimen can be controlled by adjusting the normal contact stiffness $k_n$. And corresponding to the H-M model, it is to adjust the shear modulus $G$. Adjusting the value of $k_n$ / $k_s$ for the linear contact model corresponds to the poisson's ratio $\nu$ in the H-M model, and adjusting the particle friction coefficient value $\mu$ in extent to control the peak intensity of the soil sample is common for two kinds of models.
During simulating the triaxial test on standard sands[13], it is necessary to continuously adjust \( k_n \), \( k_s \), \( k_n / k_s \) and \( \mu \) or \( G \) to make the macro-mechanical performance of the numerical sample gradually approach the actual standard sand results. After several tests, the corresponding ideal combination of mesoscopic parameters can be found for the linear contact model and the H-M model. The specific values are listed in the table 4.

Table 4 Mesoscopic parameters for linear contact model

| \( k_n \) (Pa) | \( k_s \) (Pa) | \( \mu \) |
|----------------|----------------|---------|
| 1.5e8          | 0.5e8          | 0.5     |

Table 5 Mesoscopic parameters for H-M contact model

| \( G \) (Pa) | \( \nu \) (Pa) | \( \mu \) |
|-------------|---------------|---------|
| 3.5e11      | 0.35          | 0.5     |

The macro-mechanical response curves of numerical samples obtained using two different contact stiffness models are plotted with the test results of standard sands. The analysis results show that numerical simulation can better reproduce the characteristics of strain softening and volume expansion of dense sand under drainage and shearing conditions, the macro-mechanical response trend obtained by numerical simulation is consistent with the results of laboratory tests in the changing trend.

It also can be found that the stress-strain curves obtained from the numerical simulation fluctuate in the strain softening section after the peak strength, resulting in a non-smooth curve. This is mainly because the strain softening would be accompanied by the occurrence of strain localization and result in uneven stress distribution in the sample.

![Figure18. Comparison between results of PFC2D simulations and lab tests on sands](image)

5. Summary
The paper first adopted the two-dimensional particle flow method in the particle discrete element to establish the PFC2D model of the basic test of soil mechanics simulating the plane strain experiment, that is the confined biaxial test, and then discussed the effects of the macro-mechanical response of the sand sample for two different contact stiffness models; Finally, the conventional triaxial test results of standard sands were simulated and the test results were compared and analyzed. the main contents are as follows:

(1) Linear contact model related
In the linear contact model, the relationship between the stress-strain, volumetric strain-axial strain of sands under different confining pressures, as well as the fabric and deviatoric stress, the phase transformation porosity ratio and the corresponding normal stress were all discussed separately. And the effects of changes in the macro-mechanical properties of sands under the influence of gravity,
friction coefficient, particle contact stiffness, particle size ratio, and particle shape coefficient were discussed separately.

(2) H-M contact model related
In the H-M contact model, the effects of the mesoscopic shear modulus G, the coefficient of particle friction, and the mesoscopic poisson's ratio on the macro-mechanical properties of the specimen were discussed.

(3) Comparison of linear contact model, H-M contact model and actual triaxial test
When simulating the results of a conventional triaxial test of standard sand, for a certain confining pressure level condition, both the linear contact model and H-M contact model can be used to obtain satisfactory results.

Through the analysis of the parameters for the confined biaxial test, it is concluded that in the linear contact model, the peak strength, volume change, fabric, and phase transformation stress ratio of "sand" are all subject to the "sample" confining pressure level, particle friction coefficient, and the particle stiffness ratio and particle shape coefficient, but are less affected by the "particle size ratio". In the H-M contact model, the mechanical behaviors are related with the properties of particle stiffness which include normal stiffness and shear stiffness, and less affected by poisson's ratio, while the stiffness ratio in the linear contact model is directly related to the poisson's ratio in the H-M contact model.

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