Discrete element simulation and parameter selection about triaxial test of cohesive soil containing calcareous nodules

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Abstract. Based on the discrete element method, the relationship between the microscopic parameters and the actual macroscopic parameters is introduced. In this paper the method of calculating the corresponding microscopic parameters of cohesive soil containing calcareous nodules is discussed, and the numerical model is established by using the solved parameter results. Numerical simulation results show that: the numerical model of cohesive soil containing calcareous nodules is basically consistent with the stress-strain curve of the actual triaxial test results, and has a high similarity. On this basis, the mechanism of the effect of calcareous nodules on the mechanical properties of soil on the mesoscale scale can be further discussed.

1. Preface
At present, in the triaxial compression test of geotechnical materials at home and abroad, the effect of mesoscopic structural elements on the failure morphology and physical and mechanical characteristics of geotechnical materials on macro scale is mainly considered. However, the commonly used physical tests and testing methods are difficult to analyze the meso-mechanical parameters of materials, and can not well reveal the deformation and failure of materials and the interaction mechanism between particles.

Cohesive soil containing calcareous nodules is a special regional "soil-rock mixture", which is not only different from the general ideal elastic and plastic materials, but also quite different from the general clay. It is a heterogeneous and discontiguous material. The interaction between calcareous nodules and fine particles in soil affects the physical and mechanical properties of materials. With the development of computer technology, a numerical simulation method based on the idea of discontinuous numerical simulation, discrete element method (DEM), plays a more and more important role in the study of soil-rock mixture [1]. Compared with the traditional physical experimental methods, the numerical simulation method needs less manpower and is repeatable. More importantly, it has natural advantages in the study of mechanical parameters of mesoscopic particles. Therefore, with the help of PFC3D software and particle flow method, the sample model is established to simulate the triaxial compression test of cohesive soil containing calcareous nodules.

2. Construction of triaxial test model of cohesive soil containing calcareous nodules
There are three basic units of discrete element simulation program PFC3D, which are wall, ball and contact. As a boundary, the wall acts as a constraint to ensure the basic form of the discrete element, and forms a complete whole by establishing contact[2].
2.1 Construction of particles
The calcareous nodules used in this experiment are approximately ellipsoid and the surface is uneven, so according to the size of the calcareous nodules used in the experiment, 3 three-dimensional spheres are used to form the clump as calcareous nodules shown in Figure 1.

![Figure 1. Cluster particle model of calcareous nodule](image)

The number of discrete units will affect the efficiency and results of the simulation, and if the number of spheres is too large, the computational efficiency will be greatly reduced\(^3,4\). According to the study of the size effect of particle flow simulation by Yin X T\(^5\) Liu H T\(^6\), it is known that if the ratio of the minimum discrete unit particle size to the height of triaxial specimen (\(d_{\text{min}}/D\)) is less than 0.01, the number of discrete elements would have no effect on the calculation results. Therefore, the radius range of soil particles is set to be 0.8-1.8mm in this simulation.

2.2 Construction of exposure

![Figure 2. Discrete element contact model](image)

All the particle elements in the soil are rigid bodies, and the contact between them is approximate to point contact, so it is necessary to set up the contact relationship between the elements. In the model of this test, the only contact is the contact between fine particles and nodules in soil. The soil is silty clay, and there is bond between the two kinds of contact, so we use the contact viscosity model, as shown in Figure 2. The contact strength between the fine particles in the soil and the calcareous nodules are set respectively. It is regarded as the destruction of the contact relationship and bonding contact failure if the tension in any direction between the particles in the compression process is greater than the contact strength set by the particles.

2.3 Selection of particle parameters

In the discrete element numerical simulation, the compression deformation characteristics of the initial elastic deformation stage are mainly determined by the stiffness of the particles. By calculating the triaxial model of particles with different stiffness, the shear strength-strain diagram is established, such as Fig 3, it can be found that the shear strength is proportional to the strain, and the linear slope is the elastic modulus. Through Fig 3, the functional relationship between elastic modulus and particle stiffness can be established. Therefore, by calculating the elastic modulus of the model sample in the laboratory test, and then through the relationship between the elastic modulus and the particle stiffness, the stiffness parameters of the simulated particles can be calculated.
Figure 3. Strain curve of shear strength with different particle stiffness

The macroscopic friction coefficient $\mu$ of the sample is equal to the tangent of its internal friction angle $\phi$.

$$\mu = \tan \phi$$

(1)

There is a functional relationship between the fine friction coefficient $\mu_i$ of the particles and the macroscopic friction coefficient $\mu$ of the sample.

$$\mu = 0.89367\mu_i - 0.02199$$

(2)

Figure 4. Curve of the relationship between the simulated friction coefficient and the slope $c-c_i$

When the meso-friction coefficient $\mu_i$ is fixed, there is a linear relationship between the cohesion $c$ and the contact strength $c_i$, and the slope of the $c-c_i$ line is proportional to the meso-friction coefficient $\mu_i$. The relationship between $c-c_i$ line slope and meso friction coefficient $\mu_i$ is established, as shown in figure 4. The functional relationship between $c-c_i$ line slope $S_{c-c_i}$ and meso friction coefficient $\mu_i$ can be obtained by numerical fitting.

$$S_{c-c_i} = 5.4034e^{-5.8973\mu_i}$$

(3)

Therefore, according to formula 2 and formula 3, the fine friction coefficient $\mu_i$ and contact strength $c_i$ of particles can be obtained.

The items of soil particles can be obtained by calculating the results of plain soil samples. However, because of the irregular shape of calcareous nodules, it is difficult to accurately measure the corresponding mechanical parameters in laboratory tests, but because of the great difference between the physical and mechanical properties of calcareous nodules and soil fine particles, the strength of calcareous nodules is equivalent to that of soft rock. Therefore, we can refer to the empirical value of block stone in the numerical simulation of soil-rock mixture in reference [7-10].

2.4 Construction of walls

In PFC$^{3D}$ software, the walls are all planar non-curved surfaces, so the approximate cylinders composed of several planes are used as the lateral boundary of the specimen. Two planes are added as the loading plate above and below the lateral boundary, and the middle of the loading plate is the test space. The compression process is realized by controlling the moving speed of the loading plate.
2.5. Model Construction
The soil particle unit is put into the space composed of the cylindrical wall and the loading plate, and then the cluster particles acting as calcareous nodules are placed in the position which is the spatial coordinates, and finally the soil particle units overlapping with the calcareous nodules are deleted. Fig. 4.14 is a discrete element numerical model with different locations and numbers of nodules.

3. Discrete element simulation results
Taking the PFC3D simulation results of each model specimen under confining pressure 100kPa under 21% moisture content as an example, the corresponding stress-strain curves are drawn, as shown in figure7(a). It can be seen that under 21% moisture content, with the increase of the number of nodules and the movement of the location of nodules to the center of the sample, the greater the principal stress difference of the specimen is. The stress-strain curve will also fluctuate in the stage of plastic deformation because the specimen contains nodules, and the number of nodules is positively correlated with the fluctuation range. The stress-strain curves of the above discrete element numerical simulation results are consistent with the experimental results under the same indoor conditions, as shown in figure7 (b), indicating that the existence of calcareous nodules does improve the strength of the samples.

Further combined with figure 8 (represented by the upper corner standard ' as a numerical model), the comparison of the stress-strain curve and principal stress difference between the S and B models under 21% moisture content and 100kPa confining pressure, and the measured data can be seen:
Figure 8. Comparison of numerical simulation results with laboratory tests

- in the curve shape, the numerical fitting results are in good agreement with the indoor fitting results, but the numerical model is more consistent with the hyperbolic shape, and the numerical models of BB and BC in figure 7 show the trend of strain softening under the confining pressure of 100kPa.
- under low confining pressure, the failure principal stress difference of the numerical simulation results is basically consistent with the failure principal stress difference of the test results, but with the increase of confining pressure, the failure principal stress difference of the numerical model will be slightly higher than that of the laboratory test results. According to the calculation of Mohr-Coulomb criterion, it is known that the internal friction angle of the numerical model is slightly higher than that of the test sample.

The reason for the above difference is that the numerical simulation constitutive model can not match the constitutive relation of the actual model specimen perfectly, and the second reason is that the stress history of the specimen will determine the shape of the stress-strain curve to a certain extent.

4. Conclusion

To sum up, the stress-strain curve of the discrete element simulation results of cohesive soil containing calcareous nodules in this paper is closer to the hyperbolic shape, but it is basically consistent with the characteristics reflected by the laboratory test results, and the difference of principal stress is also basically equal. Therefore, it is right to further discuss the effect of calcareous nodules on the mechanical characteristics of soil on the meso-scale based on the discrete element numerical model established according to the parameter selection method in this paper.

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