Influence of Particle Shape on Mechanical Properties of Coal Measure Soil by Discrete Element Method

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Abstract. On the basis of the discrete element theory, PFC3D was used to generate five particle models of different shapes. The impacts of particle shape on the macroscopic physical and mechanical properties of soil mass were analyzed through the numerical simulation of triaxial test as well as from a microscopic point of view. The results showed that the shear strength of irregularly shaped particles is higher than that of spherical particles, and that among the irregularly shaped particles, the shear strength of cylindrical particles is higher than that of ellipsoidal particles. Since spherical particles are associated with relatively large rotation angles during loading, samples have obvious dilatancy. However, among the irregularly shaped particles, since the inter-particular interlocking is strong and the rotation angles are relatively small, samples does not display significant dilatancy. The more irregular is the particle shape, the greater will be the energy dissipated by damping, indicating that the lesser is the kinetic energy stored in samples, the less likely the particles will move, and the more stable the sample will be.

1. Introduction
Particle shapes impose direct impacts on the macroscopic mechanical properties of particulate matter and are closely correlated to such properties of particulate matter as strength, friction, flow, and accumulation. At present, the geometrical shape of most particles in discrete element method is round or spherical. Both geometries are quite different in shape from the actual particles and have the disadvantage of having a high tendency to roll, thus the actual interlocking among particulate matters cannot be reflected. Therefore, there always are certain differences between the results of numerical simulation based on discrete element and the mechanical properties of the actual particulate matters [1-4]. Simulations involving irregular geometries of particle medium with combined particle unit have been widely used [5-7]. The combined particles are also known as clumped particles. Since there is no force between the basic elements of such a combined particle, it can be regarded as a rigid body. Combined particles of different shapes have been accurately constructed by adopting regular particle units of different sizes, quantities, and levels of tessellation. Besides, the contact calculations of particle units are based on regular particles, thus the calculations are simple. In this paper, the coal measure soil slope of a highway project in southwest Jiangxi Province was taken as the engineering background, and clumped particle units were used to simulate the irregular geometry of the particle medium, the influencing mechanism of particle shapes on the shear strength, coordination number, and porosity of particle medium were calculated and analyzed by establishing a three-dimensional (3D) triaxial compression numerical test model, and the variation pattern of the energy dissipated by damping during the simulation test were discussed.
2. Establishment of Discrete Element Numerical Model for Triaxial Test

PFC, a particle flow analysis application, was used as the computing platform, and the programming was written in Fish language. The clump templates in five different shapes were generated, as shown in figure 1. Next, by applying the template into the wall, and by generating the numerical model samples for the triaxial test using the control parameters, the microscopic parameters of the particles were set, and the servo control were applied into the model. The numerical model for triaxial test is shown in figure 2.

![Figure 1. Geometric templates of 5 particles of different shapes.](image1)

![Figure 2. Numerical calculation model of triaxial test: (a) Wall under simulated triaxial test loading, (b) Particle model generated by PFC.](image2)

Five groups of numerical model for the triaxial test could be generated according to the templates with five different shapes. The same particle size, parameters, confining pressure, and servo mechanism were set to the five groups of numerical model with different particle shapes. The density, porosity, grain composition, and other parameters of the coal measure strata for this engineering project were selected as the model parameters. The microscopic parameters of the numerical models for triaxial test are shown in table 1.

3. Analysis of Simulation Test Results

3.1. Influence of Particle Shape on Deviatoric Stress and Axial Strain of the Specimen

In order to study the influencing mechanism of different particle shapes on the deviatoric stress and axial strain of the test specimen, a confining pressure of 1.2 MPa was applied to the five numerical model groups in a unified manner. The calculation results of the deviatoric stress and axial strain are shown in figure 3.
Table 1. Mesoscopic parameters of triaxial test.

| Parameter                                      | Value             |
|------------------------------------------------|-------------------|
| Particle density                               | 2200 kg/m³        |
| Porosity                                       | 0.35              |
| Friction coefficient                           | 0.3               |
| Model particle size                            | 0.12~0.18         |
| Normal and tangential stiffness of particle contact | 1×10⁷ N·m⁻¹   |
| Damping factor                                 | 0.7               |
| Wall stiffness                                  | 1×10⁸ N·m⁻¹       |

Figure 3. Deviatoric stress and axial strain curve.

According to figure 3, the sequence of the test models in the descending order by curve peak value is as follows: Double, Four, Three, Five, and Single. The deviatoric stress of the double model grew faster; and Double model reached the stress model in a shorter time. The deviatoric stresses of the Five and Single models showed no significant decrease after peaking, which explains why the curves became stable. Nevertheless, the deviatoric stress of the Three and Four models would decrease after peaking; and the stresses of both models gradually became stable after reaching a certain value.

Samples were taken and loaded under the confining pressures of 0.8, 1.2 and 1.6 MPa to obtain the corresponding maximum axial compressive stresses, which was fitted via programming with MATLAB. The cohesion and friction angle of the samples (as shown in table 2) were obtained.

Table 2. Values of cohesion and internal friction angle.

| Model  | Single | Double | Three | Four  | Five  |
|--------|--------|--------|-------|-------|-------|
| Cohesion (KPa) | 4.9    | 53.2   | 46.6  | 56.3  | 30.31 |
| Internal friction angle (°) | 24.18  | 32.34  | 31.11 | 32.22 | 28.39 |

It can be seen from table 2 that the cohesion and internal friction angle of Single model were smaller than those of irregular particle models, but the internal friction angle and cohesion of the Double and Four models were greater. According to the analysis from a microscopic point of view, the stronger the interlocking between the particles, the greater the constraint between them, viz., the less likely particles will rotate, the more compact the sample will be, and the greater the internal friction
angle of samples will be.

3.2. Influence of Particle Shape on Porosity and Coordination Number of the Specimen

Figure 4 shows the variation curves of the porosities of the model specimen during the numerical simulation of the triaxial test. As shown in figure 4, during the initial loading, the confining pressures and axle loads increased slowly, and the porosities of particles changed slowly as well. After the loading has been conducted for a certain time length, the porosities decreased greatly. After the loading, the porosities of the Single particle model was the highest, but then plummeted to the lowest point before bouncing back up; the porosities of the other four kinds of clumped particles were relatively low, and did not bounce back up after the drop; the initial porosities can be arranged in a descending order as follows: Five, Four, Three, Single, and Double, while the porosities after the loading in a descending order are as follows: Single, Five, Double, Four, and Three.

Figure 5 shows the variation curves of the coordination numbers during the numerical simulation of the triaxial test. As shown in the figure, the coordination numbers of the calculation models of particles with different shapes increased with the lengthening of time steps. Also, the coordination numbers of the models of particles with different shapes were different before loading and had no obvious change during the initial loading. After the loading has been applied to a certain extent, the coordination numbers gradually became stable. After the test, the coordination numbers could be arranged in the descending order as follows: Five, Four, Three, Double, and Single. In other words, the larger the particle, the greater the corresponding coordination number, with the coordination numbers of clumped particles being much greater than that of single particles.

![Figure 4. Change of porosity of model particles.](image)

![Figure 5. Change of particle coordination number in the model.](image)

3.3. Analysis of Energy Dissipated by Particle Damping

Particles dissipate kinetic energy during sliding, rolling, collision, and friction, before the model finally reaches stability. However, the kinetic energy stored in the samples would drive the particles into motion. After the damping was set to 0.7, the monitoring results of energy dissipated by the damping of the samples of particles with different shapes are shown in figure 6.

According to figure 6, the more irregular the particle shape, the higher the energy dissipated by damping. Particles in the Single model dissipated the least energy. Since particles dissipate energy during sliding and rolling, it can be concluded from practical experience that the friction coefficient during rolling is smaller than that during sliding and the energy dissipated during rolling is also lower than that dissipated during sliding. In the Single samples, the energy dissipated by damping was lower. Undissipated kinetic energy may also drive the particles into motion. Since the movement of particles mainly includes rolling and sliding, the particle porosities may bounce back up after reaching its
minima, resulting in dilatancy. In irregular particle clusters, however, since the damping of samples dissipates more energy, the lesser residual energy limits the movement of particles, resulting in higher stability of the samples.

![Figure 6. Particle damping dissipation energy variation of the model.](image)

4. Conclusions
The shapes of soil particles have great influence on the mechanical properties of the samples. The cohesion and friction angles of irregularly shaped particles are greater than those of spherical particles. Irregularly shaped particles have better mechanical properties and higher strength. However, since spherical particles and needle-shaped particles have smaller cohesion and friction angles, the shear strengths of the models are lower and the mechanical properties are poor.

When external forces are loaded, the coordination number of soil particles gradually increases and the porosity gradually decreases; the samples gradually become more compact and the carrying capacity increases. Since the constraints between spherical particles are small, spherical particles induce obvious movements and rotations, causing significant dilatancy in samples. Irregularly shaped particles, however, do not have obvious dilatancy, so they will become more compact, and its samples will have better mechanical properties.

When a certain amount of energy is stored, the higher is the energy dissipated by particle damping, the lesser the kinetic energy stored in particles will be, and the less likely particles will move. Since spherical particles themselves dissipate less energy, excessive kinetic energy will constantly drive the particles into motion, resulting in obvious dilatancies in the samples.

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