Study on Physical and Contact Parameters of Limestone by DEM

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Abstract. Based on discrete element theory, a discrete element model was built to simulate the motion of single particle or particles, which provides some feasible and effective methods for determining the physical parameters and contact parameters of the discrete element model, and improves the authenticity and reliability of the material discrete element simulation. This paper provides some methods for obtaining physical parameters and mutual contact parameters. The shear modulus of limestone rock was obtained by uniaxial compression test. Using limestone raw material, the collision recovery coefficient was measured in a drop test using a high-speed camera and the static friction coefficient was obtained in a sliding plate test. The physical parameters and the contact parameters of the discrete element model of limestone were determined by measuring the stacking angle of limestone particles.

1. Introduction

Discrete element analysis methods have developed rapidly in recent decades. The discrete element method is an effective numerical simulation method for solving problems involving bulk materials [1, 2] and is widely used in metallurgy, mining, and the chemical and pharmaceutical industries [3]. The discrete element method has been successfully applied in a number of practical applications to simulate the effects and mechanical processes involving particles. As the application of discrete element method expands, material dynamic parameters are required for accurate numerical simulation of real cases and situations and for utilization as an engineering tool.

In discrete element method simulation, the properties and characteristics of various materials affect the contact and collision behavior. The physical properties of the material include density, size, shape, and shear modulus. The Hertz-Mindlin (non-slip) model is the default model of discrete element simulation software and is the most widely used model to describe particle interaction [4], which it describes the interaction between particles, and between the particles and the surrounding geometry. The most important contact parameters are the elastic recovery coefficient, the static friction coefficient and the rolling friction coefficient. These parameters are obtained mainly by direct
laboratory testing and calibration of the contact parameters. Testing methods include the uniaxial compression test, slide plate test [5, 6], and material rebound test [7].

In the general case of a collision of arbitrary objects, Lv discussed three definitions of the recovery coefficient which were inconsistent, and showed the conditions required for these definitions to be equivalent. It was found that the collision recovery coefficient and the instantaneous friction coefficient changed when the incident angle was large [8]. Yang et al. [9] measured the projection distance corresponding to two different heights by adjusting the height of the collision point on the collision plate from the base to the upper surface, and calculated the recovery coefficient of the materials particles under different conditions. With hybrid rice as an example, the recovery coefficient of three rice grains were measured under different influencing factors and at different levels. Li developed a particle contact mechanics model using discrete element method and designed a series of experiments to obtain the physical and mechanical parameters of cement clinker particles [10]. In a study of the stacking angle of a pulverized coal pile, Xia et al. [11] calibrated the simulation parameters by comparing the simulation results with those of experiments based on an orthogonal method. The flow characteristics of the model improved with the calibrated parameters. In the above studies, only virtual calibration tests or a single experiment were carried out. In this paper we present a method for determining the actual test and the calibration of virtual experiments designed to obtain the physical parameters and interaction parameters of particles in various materials, to improve the discrete element simulation process.

2. Materials and methods

2.1. Basic principle and contact model of the discrete element method

The Hertz-Mindlin (non-slip) model is the default contact model of discrete element simulation software. The normal force is based on the Hertz contact theory and the tangential force is based on the work of Mindlin and Deresiewicz. The spring and damper is used to represent the contact between the particle units. The spring represents the elastic contact of the elements, and the damper represents the non-elastic contact of the particle cells. The friction between the elements is represented by a sliding block with a friction coefficient. The contact model of the particle cells (Figure 1) is an efficient and accurate means of calculating the contact forces [12-15].

From the Hertz contact theory, the normal force between the particles is:

\[ F_{\text{normal}} = \frac{4}{3} E \sqrt{R} U_n^{3/2} \]  

(1)

Where:
Where $F_{\text{normal}}$ is the normal force between the particles; $E^*$ is the equivalent elastic modulus of the particles; $R^*$ is the equivalent particle radius; $E_A$ and $E_B$ represent the elastic modulus of particle A and B, respectively; $\nu_A$ and $\nu_B$ represent the Poisson's ratio of particle A and B, respectively; $R_A$ and $R_B$ represent the radius of the particle A and B, respectively.

To calculate the indirect contact force between the particles, the distance $d$ between two particle cells can be expressed as:

$$d = |\mathbf{r}_A - \mathbf{r}_B|$$

Where $\mathbf{r}_A$ and $\mathbf{r}_B$ represent the center position vector of particle cell A and B, respectively; $d$ is the distance between the centers of the two particle cells.

The accumulation of normal direction of the two particles can be calculated as:

$$U_n = \mathbf{R}_A + \mathbf{R}_B - d$$

Where $U_n$ is the accumulation of normal direction of the two particles.

The stiffness coefficient of the two particles is:

$$k_n = 2E^* \sqrt{R^* U_n}$$

$$k_s = \left(\frac{1}{2} \sim \frac{2}{3}\right) k_n$$

Where $k_n$ is the normal stiffness coefficient of the particles; $k_s$ is the tangential stiffness coefficient of the particles. The calculation formulas can be found in the literature [16-18].

2.2. Determining the limestone property parameters

Applying the discrete element method requires a large number of physical parameters, such as the density, shape, and shear modulus of the material particles. In this paper, limestone particle size is 0mm—13mm. First, the particle size distribution and the density were measured, then the shear modulus of the limestone was derived by a uniaxial compression test.

2.3. Measurement of particle size

Due to the large number of materials, there is a concept of average particle size and particle size distribution [19]. Sieving was used to measure the particle size and particle size distribution. In this paper, the experimental limestone was sieved by the vibrating sieve machine (Figure 2) to obtain the experimental limestone particle size of 0mm—13mm.
The various particle shapes affect the flow ability, filling properties of the material, and the acting force between the particles. For the discrete element method simulation of the limestone particle model, the particles were divided into two categories based on their shape – spherical and tetrahedron (Figure 3).

The limestone density was measured by the drainage method. The limestone is weighed and then placed in a cylinder with a measured volume of water, then the combined volume is read and the volume of the limestone calculated as the difference between the two volume readings. The density of the limestone particles is then calculated according to Equation 8.

2.5. Determining the shear modulus
The elastic modulus of the material is defined as the ratio between the stress and the strain of the material during elastic deformation:
Where $\sigma$ is the normal pressure of the material, in [Pa]; $E$ is the elastic modulus of the material, in [Pa]; and $\varepsilon$ is the strain produced by the compression of the material.

In discrete element method simulation, the elastic modulus of the limestone particles has a strong effect on the accuracy of the simulation results. In this study, the elastic modulus of limestone was measured using a servo tension and compression testing machine, and cylinder sample with a diameter of 35 mm and a height of 70 mm was obtained using a standard limestone sampling device (Figure 4).

**Figure 4.** Servo tension and compression testing machine (a), and the sampling device of the limestone sample (b).

The stress of the limestone is defined as the force $F$ per unit area $S$ in the experiment, and the strain is the ratio of the stress-induced material deformation $\Delta L$ to the initial state $L$.

\[
\sigma = \frac{F}{S} \quad (10)
\]
\[
\varepsilon = \frac{\Delta L}{L} \quad (11)
\]

According to Eqs 9–11, the elastic modulus of limestone can be calculated as:

\[
E = \frac{F \cdot L}{S \cdot \Delta L} \quad (12)
\]

The shear modulus $G$ is:

\[
G = \frac{E}{2(1+\nu)} \quad (13)
\]

For the compression test, the limestone specimen was cut into a cylindrical block and placed in the servo press and loaded according to the control program. Initially, the press advanced at a rate of 5 mm min$^{-1}$. A pressure head was used to apply pressure on the limestone cylinder. When the press was subjected to a force of 5N, the press was advancing at a rate of 2 mm min$^{-1}$. The pressure increased to the maximum and then decreased once the specimen fractured. The press head then returned to its original position at a speed of 20 mm min$^{-1}$. The pressure and the compression distance were recorded to calculate the elastic modulus of the limestone specimen. The Poisson ratio of limestone was taken as 0.25 based on the literature [20]. The shear modulus of the material was calculated according to Equation 13, as shown in Table 1.
Table 1. Uniaxial compression test data sheet

| Groups | Maximum positive pressure[N] | Deformation amount[mm] | Modulus of elasticity[Pa] | Modulus of shearing[Pa] |
|--------|-------------------------------|------------------------|--------------------------|------------------------|
| 1      | 40627.8                       | 1.37                   | $5.16 \times 10^8$       | $2.07 \times 10^8$     |
| 2      | 44214.5                       | 1.32                   | $5.84 \times 10^8$       | $2.34 \times 10^8$     |
| 3      | 39863.6                       | 1.43                   | $4.85 \times 10^8$       | $1.94 \times 10^8$     |
| 4      | 46776.9                       | 1.56                   | $5.23 \times 10^8$       | $2.09 \times 10^8$     |
| 5      | 41300.1                       | 1.42                   | $5.06 \times 10^8$       | $2.02 \times 10^8$     |
| Means  | 42556.8                       | 1.42                   | $5.23 \times 10^8$       | $2.09 \times 10^8$     |

3. Measurement and analysis of the contact parameters

The contact parameters of the discrete element method model based on the Hertz-Mindlin non-slip contact model are the elastic recovery coefficient, static friction coefficient, and rolling friction coefficient. We designed a series of experiments to obtain the elastic recovery coefficient, the static friction coefficient between the particles and the steel plate, and the internal friction coefficient.

3.1. Determining the restitution coefficient of particle collision

The collision recovery coefficient is an important parameter to characterize the energy loss in a collision. Newton, Poisson, and Stronge define the collision recovery coefficients for objects from speed, impulse, and energy, respectively [21-23]. In this paper, we use the definition of Newton, expressed as:

$$ e = \frac{v_1' - v_2'}{v_1 - v_1'} $$

(14)

Where $v_1' - v_2'$ is the relative velocity after the collision of two particles, in m $s^{-1}$, and $v_1 - v_1'$ is the relative velocity before the collision of the two particles, in m $s^{-1}$.

Here, we determine the collision recovery coefficient in a collision between limestone particles, and between limestone particles and a steel plate. The coefficients were estimated from the experiment results; the experiment was based on the free fall of limestone particles which were released from a certain height (Figure 5). The particles were dropped onto a steel plate or a limestone base. The falling material was recorded at an initial height $H_0$ and the limestone collision bounce height was $H$. According to the of conservation of energy law, for a free-falling bounce height $H$, the recovery coefficient $e$, is:

$$ e = \frac{H}{\sqrt{H_0}} $$

(15)

Although the limestone particles are under the action of gravity, the process of collision rebound is still fast, and it is difficult to accurately determine the rebound height of the particles. For precise measurement of the recovery coefficient, a high-speed camera was used, combined with a test system and image processing technology that accurately tracked the particle positions during the rebound process. All the limestone particles were released from the same height.
Limestone particles with high spherical shape were used for the experiment, to avoid particle bounce in the vertical direction after a big shift. The particles fell from a height of 500 mm in free fall onto the base. The experiment was repeated 50 times and then calculated average value and the results are shown in Table 2.

Table 2. Results of limestone collision test

| Experiments          | $H_0$[mm] | $H$[mm] | Recovery coefficient |
|----------------------|-----------|---------|----------------------|
| Limestone-limestone  | 500       | 21.67   | 0.208                |
| Limestone - steel    | 500       | 165.72  | 0.557                |

3.2. Determining the coefficient of static friction

The application of discrete element method to simulate material movement involves the friction between the limestone particles and the friction between the limestone particles and the impacted surfaces. Therefore, the value of the friction coefficient will directly affect the accuracy of the simulation results. In existing discrete element method simulation programs the numerical value of the friction coefficient is often obtained from the literature rather than derived experimentally. It is not an accurate reflection of the mechanical properties of the particles. In this paper, a series of experimental methods were used to measure the friction coefficients of the limestone samples.

3.2.1. Determining of the coefficient of static friction between particles. The static friction coefficient between the limestone particles is determined by measuring the stacking angle of the particles. Generally, the coefficient of static friction between particles can be expressed by the internal friction angle of the particles. When the particle fluidity is good, the internal friction angle is considered equal to the stacking angle [24]. Thus, we calculated the static friction coefficient of the limestone particles using the particle stacking angle $\phi$ according to the following relationship:

$$\mu_1 = \tan\phi$$

The limestone particles were dropped through a fixed funnel, forming a cone-shaped pile on the horizontal surface below, and the angle formed with the horizontal surface is the stacking angle (Figure 6). To eliminate the interference between the particles and the base material, the receiving box was filled with the same material that was tested.
Figure 6. Funnel experiment device (a) and the measurement of the repose angle (b).

This experiment was repeated 10 times and the average stacking angle was calculated. The average value of $\phi$ was $37.6^\circ$ and the coefficient of static friction between the particles was 0.77.

3.2.2. Determining the static friction coefficient between the particles and the steel plate. The static friction coefficient of the limestone particles and the steel plate was measured by the ‘sliding plate’ test method. The material particles were placed on the horizontal steel plate and the plate was slowly tilted to form an angle with the horizontal plane. When the limestone fragments started sliding, the static friction coefficient between the limestone and steel plate could be calculated according to the angle between the steel plate and the horizontal plane.

In sand crushing machinery, friction occurs between the limestone particles in the rotor and between the particles and the wall of the rotor, which is made of steel. Therefore, our experiment was designed to measure the static friction coefficient of limestone particles and steel. To obtain the angle between the steel plate and the horizontal plane, we first calibrated the angle using an inclination ruler (Figure 7(a)). A plastic ring was used to contain the limestone particles on the steel plate and prevent them from scattering.

In the experiment, the limestone particles were placed on the steel plate and the plate was tilted gradually with a rotating handle. When the limestone particles in the plastic ring were about to slide down the slope, the tilting was stopped and the angle between the horizontal plane and the steel plate was recorded. The static friction coefficient between the limestone particles and the steel plate is expressed as:

$$\mu_2 = \tan \theta$$  \hspace{1cm} (17)
Where $\theta$ is the angle between the steel plate and the horizontal plane. $\mu_2$ is static friction coefficient between the limestone particles and the steel plate.

The experiment was repeated ten times, and the mean value of $\theta$ was $31.2^\circ$, and the coefficient of static friction $\mu_2$ between the limestone particles and the steel plate was 0.61.

3.3. Determining the rolling friction coefficient

In the discrete element simulation, the material and shape of the particles have a strong influence on the friction coefficient. At present, there is no material parameter database as a reference. Our experiments and their verification by numerical simulation can ensure the accuracy of the material property parameters in the calculation model. Because of the limestone particle size and contact surface in the experiment are very small, it is difficult to use the method of direct determination based on two particles or between the particles and the contact surface to estimate the rolling friction coefficient. However, the contact parameters can be calibrated experimentally, changing the experiment conditions according to the relevant local conditions. In this paper, the rolling friction coefficient of limestone particles was determined by stacking angle fitting.

![Figure 8. Determining the stacking angle: Laboratory experiment (a) and numerical simulations (b).](image)

First, a stacking angle experiment was carried out in the laboratory. The limestone particles were placed in a large cone-shaped container and then released from the same height onto a steel plate in free fall, and the stacking angle was formed (Figure 8(a)). Multiple experiments were carried out and the stacking angle was measured using an angle ruler. The average measured stacking angle was $37.2^\circ$.

In the discrete element method numerical simulation, the results are affected by various parameters such as the Poisson's ratio, shear modulus, shear modulus, density, recovery coefficient, static friction coefficient, and rolling friction factor. All these parameters were obtained in the laboratory experiments except the rolling friction coefficient. The same stacking angle experiments were carried out in the discrete element method (Figure 8(b)) and then the rolling friction coefficient was thus fitted numerically. The rolling friction coefficient between the limestone particles is 0.1 and the rolling friction coefficient between the particles and the contact surface is 0.07.

4. Parameter validation of contact model of limestone indiscrete element method

To verify the accuracy of the physical parameters calculated in the numerical simulation a ‘hollow tube’ experiment was performed and the results of the experiment and simulation were compared.
The stacking angle was measured using a hollow open steel cylinder (Figure 9). The cylinder was placed on a flat horizontal surface and filled to a certain height with limestone particles. The cylinder was then slowly lifted without disturbing the particles, and the particles spread from the bottom of the cylinder to form a conically shaped pile. The particle size was 0 mm—13 mm. The diameter of the steel cylinder was 140 mm its height was 350 mm. The weight of the load was 8 kg (equal to about 50000 particles), and the lifting speed was 0.1 m/s. The experiment was repeated a number of times. The average stacking angle was 29.9°.

The material properties and contact parameters of limestone and steel used in the discrete element method are shown in Tables 3 and 4.

| Test       | Poisson's ratio | Shear modulus[Pa] | Density[kg∙(m^3)^{-1}] |
|------------|-----------------|-------------------|------------------------|
| Limestone  | 0.25            | 2.09e+8           | 2650                   |
| Steel      | 0.30            | 7e+10             | 7800                   |

| Mutual contact | Coefficient of restitution | Coefficient of static-friction | Rolling friction coefficient |
|----------------|---------------------------|-------------------------------|----------------------------|
| Limestone—limestone | 0.208                    | 0.77                          | 0.1                        |
| limestone—steel    | 0.557                    | 0.61                          | 0.07                       |

In the EDEM simulation, using the two types of limestone particle models established in Figure 3, the particle size is randomly distributed in the range of 0 mm to 13 mm, the model was established, and the particles generation, cylinder lifting, and particles stacking were completed in four processes, as shown in Figure 10.

Using the parameters of Tables 3 and 4, a physical test and numerical simulation under the same working conditions were carried out. The repose angle calculated in the simulation using the hollow cylinder method was 30.6°. The deviation between the numerical value and the experimental results is 2.3%. This verifies that the high accuracy of the limestone and steel plate material and contact parameters obtained in the discrete element method simulation. These parameters can be used in further simulations to estimate the behavior of limestone particles in various crushing and processing machines, and provide a reference for future simulation work.
5. Conclusion

This article describes a discrete element model based on the non-slip Hertz-Mindlin contact model. The model was used to obtain the physical and contact parameters of limestone particles against a steel surface. The basic parameters such as density, friction coefficient, elastic modulus, and collision recovery coefficient were determined in laboratory experiments, providing the basis for the discrete element method simulation calculation. The results can be applied in various limestone crushing and processing machinery. The main conclusions are as follows:

(1) In the discrete element simulation, the material parameters have an important influence on the simulation results. To improve the accuracy of the simulation results, the physical parameters and contact parameters of the selected contact model can be determined by a combination of experimental and simulation tests.

(2) The mean value of the elastic modulus of limestone is $5.23 \times 10^8$ Pa, and the shear modulus is $2.09 \times 10^8$ Pa. The collision recovery coefficient between the limestone particles and between the limestone and the steel plate are 0.208 and 0.557, respectively.

(3) The experimental results for the friction coefficient among the limestone particles and between the limestone and the steel plate are as follows: the static friction coefficient is 0.77 and 0.61, respectively, and the rolling friction coefficient is 0.1 and 0.07, respectively.

(4) The good agreement and small deviation between the discrete element simulation results and the experimental results verify the reliability of the measured parameters and the numerical model.

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