Effect of microcosmic contact stiffness heterogeneity on macroscopic mechanical parameters of rock

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Abstract. The particle flow method is used to build a rock material model formed by the contact between the particles and the geometric constraints. The heterogeneous representation method of rock material components is used to describe the heterogeneous characteristics of the contact stiffness of particles, and a heterogeneous rock material model is established. This numerical model is used to perform numerical simulation experiments on the mechanical properties of rock materials. The influence of the contact stiffness heterogeneity of meso-particles on the macroscopic deformation mechanical properties of rock materials is studied herein. The law of the influence of the contact stiffness heterogeneity on the macroscopic mechanical parameters of rock materials is obtained. In addition, a dimensionless coefficient of the variation of the material parameters is introduced to define the degree of material heterogeneity used to describe the degree of heterogeneity of rock materials. The results show that heterogeneous representation method of the rock material components can be used to describe the heterogeneity of the meso-parameters of rock materials. The macroscopic deformation of the particle flow model of heterogeneous rock materials under load is elastic linear growth at the initial stage and strain-softening deformation failure at the later stage of failure. The deformation parameters of rock materials have a linear relationship with the particle stiffness, while the strength parameters have a quadratic relationship with the particle stiffness. The macroscopic mechanical parameters of rock materials are all weakened by the influence of heterogeneity. The smaller the degree of heterogeneity, the smaller the weakening effect will be. The greater the degree of heterogeneity, the greater the weakening effect.
1 Introduction

Rock materials are formed by the arrangement and the combination of several different media on a microscopic scale[1]. Rock materials have typical heterogeneous properties.

The heterogeneity of rock materials is the main factor determining the rock deformation and failure characteristics [2,3]. A large number of rock mechanical test results have shown that the physical and mechanical parameters of rock material samples have great discreteness[4]. The rock material composition and contact heterogeneity are important factors affecting the dispersion of the rock mechanical test results. At the microscopic level, rock materials are composed of medium particles. The rock material heterogeneity is mainly manifested in the difference in the physical and mechanical properties of microscopic media. The smaller the difference in the physical and mechanical properties of the microscopic media that constitute the rock materials, the better the material homogeneity of materials will be. On the contrary, the greater the difference between both, the worse the material homogeneity of materials will be. Fang used the Weibull distribution and the Fast Lagrangian Analysis of Continuum(FLAC) program to calculate the whole-process stress–strain curves of heterogeneous rock materials under different surrounding rock pressures [5]. Tang used the Weibull distribution to describe the heterogeneous characteristics of rock materials and developed rock failure process analysis systems, RFPA2D[6] and RFPA3D[7], using a material damage model. Meanwhile, Yue[8] and Chen[9] obtained bases from the color space multi-threshold region segmentation method to reconstruct the real meso-structure of rock materials and extend the method to three dimensions through the grinding and scanning circulation system. They studied the mechanical properties of heterogeneous rock materials using the finite element method. Potyondy and Cundall obtained the mesoscopic parameters of Lac du Bonnet granite[10]. Backstrom investigated the relationship between the mesoscopic simulation results and the macroscopic stress–strain curve of granite[11]. Hsieh[12] studied the deformation mechanism of sandstone. Stavropoulou[13] performed a microscopic experimental study of marble. In recent years, many Chinese scholars have also conducted studies on the rock material heterogeneity[14]. Nevertheless, most of these studies on the rock material heterogeneity were based on the continuum theory or used the macroscopic parameters of particles.

This study describes the contact stiffness heterogeneity of rock particles using the heterogeneous property description method based on the particle flow code. Numerical models are used to simulate the mechanical behavior of heterogeneous rock materials, study the macroscopic deformation mechanical properties of rock materials under different heterogeneous conditions, and reveal the influence of the heterogeneity of the microcosmic contact stiffness of rock particles on the macroscopic mechanical parameters.

2 Method for expressing the heterogeneous properties of rock materials

2.1 Heterogeneity representation method of the rock material composition

In terms of the rock material composition, a rock is a heterogeneous body composed of different mineral particle aggregates and cementing materials. Most rocks are composed of several mineral materials. The mineral composition of rocks has a very important influence on its mechanical properties and, in some conditions, can even have a decisive influence. Heterogeneity is mainly
manifested in the difference between the physical and mechanical properties of the microscopic mineral particles that constitute the rock material. The homogeneity of a rock is better when the difference of the physical and mechanical properties of the material components is smaller. Conversely, the greater the difference in the physical and mechanical properties of the material components, the worse the rock homogeneity will be.

The heterogeneity representation method of the rock material composition is based on the material group of the rock material itself, including basic properties like the type of material component and its content in the rock material. The material composition is different for different rocks. The method is based on the material composition of the rock category and the content analysis defining the category rule of the material component unit. According to the laws of using the Monte Carlo method, all units in the numerical model category judgment and assignment based on the rock composition of the material itself describe the heterogeneity of the material properties. Figure 1 depicts the basic process of using this method to establish the numerical model.

![Figure 1](image1.png)

**Figure 1.** Flow of the random parameter assignment of the rock mineral cell unit.

### 2.2 Classification determination interval of the material component particles

The heterogeneous rock used in this study was assumed to be composed of $m$ material components. The content of the Class $i$ material component is denoted by $n_i$. The following formula must be true:

\[ \sum_{i=1}^{m} n_i = 1 \]  

(1)

The cumulative content $u_i$ of the material components is calculated as follows:

\[ u_i = \begin{cases} 0 & i = 0 \\ \sum_{j=1}^{i} n_j & i = 1, 2, \ldots, m \end{cases} \]  

(2)

The material component category determination interval is defined as follows according to $u_i$:

\[ A_i = \begin{cases} [u_{i-1}, u_i) & i = 1, 2, \ldots, m - 1 \\ [u_{m-1}, 1] & \text{with } m \end{cases} \]  

(3)

This definition interval divides the interval $[0,1]$ into $m$ cells. The proportion of the interval $A_i$ in the interval $[0,1]$ is calculated as follows:
\[ P_i = u_i - u_{i-1} = n_i \] (4)

2.3 Criteria for the classification of the material component particles

The uniform distribution \([0,1]\) is adopted as the objective function according to the Monte Carlo method. The probability distribution function is presented as follows:

\[ F(x) = x \] (5)

The probability density function is

\[ f(x) = 1 \] (6)

We have the following equation for the initial random number \(\xi_k\):

\[ F(x) = \xi_k \] (7)

The target random number \(x_k\) is equal to \(\xi_k\). As shown in Figure 2, if the random number \(x_k\) is in the range \(A_i\), the material unit corresponding to the random number is determined as a Class \(i\) material component, and a corresponding parameter value is assigned.

Figure 3 shows a mechanical specimen model of the heterogeneous rock materials based on the particle flow code and the heterogeneity representation method.

3 Mechanical properties of meso-heterogeneous rock materials

3.1 Basic parameters of the model specimen

A mechanical model of heterogeneous rock materials was established based on the particle flow and heterogeneity representation methods of the rock material composition. A uniaxial compression test was then performed for the rock materials. The influence of meso-heterogeneity on the macroscopic mechanical properties of the materials was studied using the meso-contact stiffness of the material particles as the characterization. The uniaxial compression test specimen was 50 mm wide and 100 mm high. Tables 1 and 2 list the particle size and the bonding parameters of the test model.

| least radius (mm) | particle diameter ratio | density (g/cm³) | stiffness ratio | friction coefficient |
|-------------------|-------------------------|----------------|----------------|---------------------|
| 0.275             | 1.66                    | 2.63           | 2.46           | 0.50                |

| normal strength(MPa) | parallel strength(MPa) | elasticity modulus (GPa) | radius multiplier |
|----------------------|------------------------|--------------------------|------------------|
| mean value           | standard deviation     | mean value               | standard deviation |

Figure 2. Schematic diagram of sort judgment. Figure 3. Test model of an inhomogeneous rock.
3.2 Influence of meso-stiffness on the macroscopic mechanical properties of rock materials

To facilitate the analysis, we considered that the rock specimen was composed only of two types of mineral particles, with 50% content each. The contact stiffness of the first type of mineral particle remained unchanged. Only that of the second type was altered. A numerical simulation of the uniaxial compression test was subsequently performed. Table 3 presents the parameters of the normal contact stiffness $k_n$. The stiffness ratio of the normal stiffness $k_n$ and the tangential stiffness $k_s$ was 2.46.

Table 3. Normal contact stiffness for the test model.

| specimen | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|----------|----|----|----|----|----|----|----|----|----|----|----|----|
| material 1 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 | 60 |
| material 2 | 10 | 20 | 35 | 40 | 50 | 60 | 70 | 80 | 90 | 100| 110| 120|

Figure 4 illustrates the stress–strain curves of the uniaxial compression test of the model specimens of the heterogeneous rock material considering the stiffness of different particles. The numerical simulation results showed that the heterogeneous rock specimens have strain-softening deformation characteristics. The macroscopic elastic modulus and the compressive and tensile strengths of the specimens all gradually increased with the increase of the contact stiffness of the second particle type. Figures 5–7 depict the variation curve of the macroscopic elastic modulus, Poisson's ratio, and compressive strength with the normal contact stiffness of Material 2 particles, respectively. The experimental results showed that for the heterogeneous rock materials, the macroscopic deformation parameters, including the elastic modulus and Poisson’s ratio, linearly increased with the normal contact stiffness of Material 2 particles. The compressive strength increased with the normal contact stiffness of Material 2 particles in a quadratic shape, and this increase gradually decreased with the stiffness increase.

Figure 4. Uniaxial compression test stress–strain curves of the heterogeneity models.

Figure 5. Variation of the elastic modulus with normal contact stiffness.

Figure 6. Variation of Poisson's ratio with normal contact stiffness.

Figure 7. Variation of the compressive strength.
contact stiffness. with normal contact stiffness.

4 Influence of the heterogeneity degree on the macroscopic mechanical parameters

4.1 Heterogeneity degree of the rock material

The heterogeneity degree of the rock material is defined by the coefficient of variation of meso-particle parameters. For the normal contact stiffness, the heterogeneity $C_v$ is expressed as follows:

$$C_v = \frac{\sigma(k_n)}{E(k_n)}$$  \hspace{1cm} (8)

where, $C_v$ is the heterogeneity degree defined by the normal contact stiffness $k_n$ of rock particles, and $\sigma(k_n)$ and $E(k_n)$ are the standard deviation and the mathematical expectation of the normal contact stiffness of each particle in the model, respectively.

The heterogeneity degree is a dimensionless quantity that reflects the deviation rate of random parameters relative to the mean value. The larger the $C_v$, the greater the dispersion degree of the particle parameters relative to the mean value and the worse the material homogeneity. The material is a homogeneous model when $C_v$ is equal to 0.

According to the heterogeneity representation method of the rock material composition, the probability that any unit in the model is determined to be a Class $i$ material component is equal to the content of Class $i$ granular materials in the rock composition. The heterogeneity degree is calculated as follows according to Eq. (8):

$$C_v = \frac{\sigma(k_n)}{E(k_n)} \frac{\sum_{i=1}^{m} n_i k_n^i - (\sum_{i=1}^{m} n_i k_n^i)^2}{\sum_{i=1}^{m} n_i k_n^i}$$  \hspace{1cm} (9)

where $m$ is the number of material components, and $\sigma(E_i)$ and $E(E_i)$ are the standard deviations and the expected values of each material component parameter in the numerical model, respectively.

4.2 Influence of the rock material heterogeneity degree

Table 4 lists the normal contact stiffness parameters used in the uniaxial compression test based on the particle flow method considering that the rock specimen is only composed of two types of mineral particles with 50% content each. The stiffness ratio of the normal stiffness $k_n$ and the tangential stiffness $k_s$ was 2.46. The heterogeneity degree of the model was calculated according to Eq. (9).

Table 4. Normal contact stiffness for the test model.

| specimen | 1  | 2  | 3  | 4  | 5  | 6  |
|----------|----|----|----|----|----|----|
| material 1 | 10 | 20 | 30 | 40 | 50 | 60 |
| material 2 | 110| 100| 90 | 80 | 70 | 60 |
| heterogeneity degree | 0.83 | 0.67 | 0.50 | 0.33 | 0.17 | 0 |

Table 4 shows that Sample 1, with the largest heterogeneity degree, had the largest difference in the particle contact stiffness among the six specimens. The Material 1 particle in Sample 6 was the same as that in Material 2, which comprised homogeneous rock materials with zero heterogeneity.

The number of macroscopic parameters (e.g., elastic modulus, Poisson's ratio, and compressive
strength of each specimen) was calculated according to the numerical test results. Figures 8–10 illustrate the relationship curves between each parameter and heterogeneity.

Figures 8–10 show that when the heterogeneity degree of the rock material was defined by the coefficient of variation, the dispersion type of the meso-contact stiffness of the rock material particles gradually increased with the heterogeneity increase. The macroscopic elastic modulus, Poisson's ratio, and compressive strength of the rock material also gradually decreased. When the heterogeneity was small, the number of macroscopic parameters gently decreased. In contrast, when the heterogeneity was large, the number of macroscopic parameters gradually decreased. This is because when the heterogeneity degree is small, the differences in the physical and mechanical properties of the mineral particles of the rock materials are small, and their stress and deformation characteristics are similar. The macroscopic physical and mechanical properties of materials are relatively less affected by their heterogeneity. When the heterogeneity degree is bigger, the material particles of the physical and mechanical characteristic difference are bigger. Under the same load condition, the difference in the particle displacement change is bigger and further affects the particle loading. The material can balance the larger load distribution within the system, showing that the macro physical and mechanical parameters of rock materials are affected by the anisotropic properties.

**Figure 8.** Variation of the elastic modulus with the heterogeneity degree.  
**Figure 9.** Variation of Poisson's ratio with the heterogeneity degree.  
**Figure 10.** Variation of the compressive strength with the heterogeneity degree.

### 5 Conclusions
The following conclusions were derived from this study:

1. The heterogeneity representation method of the rock material composition can be used to describe the heterogeneity of the meso-parameters of the rock material according to the material composition and the content of the rock material itself.

2. The macroscopic deformation of the particle flow model of the heterogeneous rock materials under load is elastic linear growth at the initial stage and strain-softening deformation failure at the later stage of failure.
(3) The elastic modulus and Poisson's ratio of heterogeneous discontinuous rock materials have a linear relationship with the particle stiffness, while the compressive and tensile strengths have a quadratic relationship with the particle stiffness.

(4) The macroscopic mechanical parameters of the rock materials are all weakened by the influence of the heterogeneity. The weakening effect of the macroscopic parameters is smaller when the degree of heterogeneity is smaller. In contrast, the weakening effect of the macroscopic parameters is larger when the degree of heterogeneity is larger.

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