Calibration of Microscopic Mechanical Parameters of Granite Using Actual Distributions and Orthogonal Simulations

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Abstract The purpose of the paper is to investigate a calibration technique for the microscopic mechanical parameters of the granite. The video images photographed during the laboratory test were used to determine the actual types and locations of various compositions. The grains and cements of the compositions were then assumed to be assembly of particle disks and parallel bonds. The pixel and particle loops were combined to set the actual compositions in simulation. Using the micro-mechanical parameters in a four level, thirty-two orthogonal tests were conducted to examine the sensitivity of the micro-mechanical parameters on the macro ones. A practical method was thereafter proposed to determine the micro-mechanical parameters using laboratory test results. It shows that the elasticity, Poisson's ratio and strength were much correlated between micro-macro scales; the convergence was much quickly if considering the actual distributions of compositions and orthogonal simulation results.

1 Introduction

A rock is generally composed of various compositions. The types and interactions between these compositions may much affect the micro mechanical properties and then control the macro features of the rock material. The indices reflecting the types and interactions between compositions can be represented by the mechanical parameters in the micro-scale.

In recent years, a lot of approaches had been made to determine the micro mechanical parameters of a rock, mostly focusing on the combination of the particle flow simulation and calibration technique based on the laboratory tests. For example, Potyondy and Cundall [5] investigated micro mechanical parameters of the Lac du Bonnet granite using a parallel-bonded model (PBM) and numerical simulations; Hsieh et al. [2] examined the relations between the percentages of

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micro compositions with the macro properties of the sandstone; Xu et al. [7] obtained the micro parameters of a limestone. Some researchers try to extract the composition distributions using the digital image processing, in which the binarization technique was mostly used. For example, Xu et al. [9] examine the micro features of a soil-rock mixture using the binarization technique; Ding et al. [1] developed a particle simulation model for bi-axial test of a soil-rock mixture using the binarized images.

The elementary aspect in estimating the mechanical properties of a rock using numerical simulation is the determination of the microscopic mechanical parameters, which were much dependent on the actual distributions of the micro compositions. In the existing approaches, as we know, the actual distributions were less accounted for. Moreover, the general-used binarization technique was not suitable to the materials composed of more compositions. In the current study, taking the Beishan granite as an example, the actual distributions were determined using the digital image processing and utilized as the input data in particle simulation. The orthogonal simulation tests were then used to determine the micro-mechanical parameters in simulating the macro properties based on laboratory tests. A new calibration technique for estimating the microscopic mechanical parameters were also proposed.

2 Determination of Actual Types and Positions

The most important aspect in determining micro parameters is to examine the relations between macro and micro parameters. For this purpose, the video image processing techniques were conducted to determine the actual types and positions while the orthogonal simulations were used to explore the macro-micro relations.

The video images were photographed during the laboratory uni-axial compression tests. A frame at any time was then extracted. The extracted frame was colorful and converted into grayscale one (Fig. 1). The sizes of the specimen were 49.9 mm in width and 99.9 mm in height. Conventional mineral identification technique was used to determine the thresholds between various minerals. In the current study, the distinguished thresholds of biotite-quartz, quartz-feldspar was 87 and 202, respectively. These thresholds were used to determine the mineral type of each pixel in the specimen image. The actual coordinates were then computed based on the relation between the sizes of total pixels and whole specimen.

Nevertheless, if the type of individual pixel was used as input in particle flow simulation, the occupied memory was too great. To balance the simulation time and the memory used, the neighborhood average technique (with the size of 3×3 pixels) and sequential interlacing sampling were conducted.

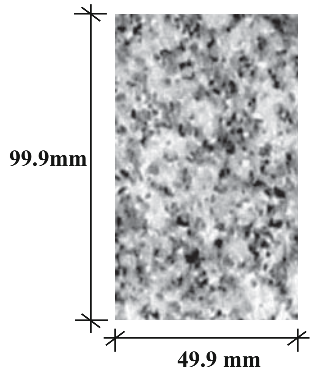

Fig. 1 A frame of granite specimen

3 Orthogonal Simulations

3.1 Geometry of Particle Flow Simulation

In the current study, the virtual distributions were established using an integration code package (Augmented FishTank) of the Particle Flow Code in 2-Dimensions (PFC2D) developed by the Itasca Consulting Group [4]. The grains were assumed as disks, whereas the cements were assumed as parallel-bonds. All of the particles were randomly generated with a minimum radius of 0.50 mm and a ratio of the maximum to minimum radius being 1.66. The density of the particle was taken as 2630.0 kg/m^3. The existing particles were then set to the type of the nearest pixels obtained from the image processing results. All of the existing particles were set by the particle and pixel loops. This method is much suitable to a material composed of more than two compositions with arbitrary shapes. The geometry of the specimen in the particle flow simulation is shown in Fig. 2.

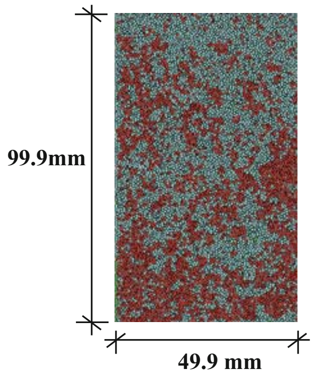

Fig. 2 Specimen geometry in particle flow simulation

3.2 Initial Micro Mechanical Parameters

The initial calibration was performed according to the correlations of the elasticity modulus, stiffness ratio and strength between macro and micro scales [7, 10]. The micro mechanical parameters were set as follows: (1) for grains, elasticity modulus $E_P = 3.10$ GPa, stiffness ratio $k_{nP}/k_{sP} = 2.00$, friction coefficient $\mu_P = 0.30$; (2) for parallel bonds, elasticity modulus $E_C = 2.85$ GPa, stiffness ratio $k_{nC}/k_{sC} = 2.50$, average normal strength $\sigma_C = 23.01$ MPa, average tangential strength $\tau_C = 22.85$ MPa. The corresponding macro parameters were: elasticity modulus $E_2 = 3.10$ GPa, Poisson's ratio $\mu_2 = 0.243$, strength $\sigma_2 = 31.318$ MPa. The PFC simulated results were represented by the elasticity modulus E_1, Poisson's ratio μ_1, and strength σ_1. The summation of the squared relative errors is

$$\delta = [(E_1 - E_2)/E_1]^2 + [(\mu_1 - \mu_2)/\mu_1]^2 + [(\sigma_1 - \sigma_2)/\sigma_1]^2 = 0.00118$$

Because 0.00118 is relatively small, these micro parameters were assumed as the fundamental ones in the orthogonal simulations. The contact parameters of the feldspar-feldspar were taken as fundamental contact properties, the parallel mechanical parameters of the quartz-quartz and biotite-biotite contacts were respectively set to 1.0 and 0.4 times of those between feldspars. Other parallel mechanical parameters were taken as the average amounts of contacted particle-pairs.

3.3 Orthogonal Simulations

The orthogonal simulations were then used to investigate the macro-micro correlations. In the orthogonal simulations, seven micro mechanical parameters and four level of each parameter were considered. The seven micro parameters include: (1) elasticity modulus E_P, stiffness ratio k_{nP}/k_{sP}, and friction coefficient μ_P of particles; (2) elasticity modulus E_C, stiffness ratio k_{nC}/k_{sC}, and average amounts of normal strength σ_C and tangential strength τ_C of parallel bonds. No interaction between these micro parameters was considered and a orthogonal table $L_{32}(4^9)$ was selected (where 32, 4, and 9 represent times of the simulations, levels of the factors, and number of considered factors, respectively). Seven above-mentioned factors were used as the micro parameters. Four levels were the magnitudes increased to 120, 100, 80, and 60 % from the fundamental ones.

4 A Proposed Method to Determine Micro Parameters

4.1 Sensitivity Analysis of Macro-Micro Parameters

The range and variance analyses were also performed using the orthogonal simulation results. To perform the range analysis, each of the macro simulation parameters (E, μ, or σ) was used as response values to estimate the influencing magnitude of micro parameters or factors.

The results in the range analysis are shown in Table 1. From Table 1, it can be seen that: (1) As for elasticity modulus of the specimen, the optimal levels of order of micro parameters are $(E_P)_1 - (k_{nP}/k_{sP})_1 - (\mu_P)_3 - (E_C)_1 - (k_n/k_s)_4 - (\sigma_C)_3 - (\tau_C)_2$, and primary order is $E_C - E_P - k_n/k_s - k_{nP}/k_{sP} - \mu_P - \tau_C - \sigma_C$; (This means that the elasticity modulus has a good correlation between micro and micro scales.) (2) As for Poisson's ratio of the specimen, the optimal levels of order of micro parameters are $(E_P)_1 - (k_{nP}/k_{sP})_3 - (\mu_P)_1 - (E_C)_4 - (k_n/k_s)_1 - (\sigma_C)_2 - (\tau_C)_4$, and primary order is $k_n/k_s - E_P - k_{nP}/k_{sP} - E_C - \mu_P - \sigma_C - \tau_C$. (This means that the Poisson's ratio has a good correlation between micro and micro scales); and (3) As for the strength of the specimen, the optimal levels of order of micro parameters are $(E_P)_1 - (k_{nP}/k_{sP})_3 - (\mu_P)_1 - (E_C)_4 - (k_n/k_s)_2 - (\sigma_C)_1 - (\tau_C)_2$, primary order is $\sigma_C - \tau_C - \mu_P - (E_C) - k_{nP}/k_{sP} - E_P - k_n/k_s$. (This means that the strength has a good correlation between micro and micro scales.) Therefore, the elasticity modulus, Poisson's ratio and strength have a good correlation between micro and micro scales.

The results of the variance analysis were listed in Table 2. It can be seen that (1) The macro-micro parameter pairs with highly significances are: $k_{nP}/k_{sP} - \sigma$, $\mu_P - \sigma$, $E_C - (E,\sigma)$, $k_n/k_s - \mu$, $\sigma_C - \sigma$, $\tau_C - \sigma$; and (2) The macro-micro parameter pairs with medium significances are: $k_{nP}/k_{sP} - \mu$, $k_n/k_s - \sigma$, and E_P—all of three macro parameters.

Table 1 Range analysis results based on orthogonal simulations

Macro parameters	Optimal levels of order	Primary order
Elasticity modulus	$(E_P)_1 - (k_{nP}/k_{sP})_1 - (\mu_P)_3 - (E_C)_1 - (k_n/k_s)_4 - (\sigma_C)_3 - (\tau_C)_2$	$E_C - E_P - k_n/k_s - k_{nP}/k_{sP} - \mu_P - \tau_C - \sigma_C$
Poisson's ratio	$(E_P)_1 - (k_{nP}/k_{sP})_3 - (\mu_P)_1 - (E_C)_4 - (k_n/k_s)_1 - (\sigma_C)_2 - (\tau_C)_4$	$k_n/k_s - E_P - k_{nP}/k_{sP} - E_C - \mu_P - \sigma_C - \tau_C$
Strength	$(E_P)_1 - (k_{nP}/k_{sP})_3 - (\mu_P)_1 - (E_C)_4 - (k_n/k_s)2 - (\sigma_C)_1 - (\tau_C)_2$	$\sigma_C - \tau_C - \mu_P - (E_C) - k_{nP}/k_{sP} - E_P - k_n/k_s$

Table 2 Significances after variance analysis based on orthogonal simulations

Factors	E_P	k_{nP}/k_{sP}	μ_P	E_C	k_n/k_s	σ_C	τ_C	Others
E	Medium	No	No	Highly	No	No	No	No
μ	Medium	Medium	No	No	Highy	No	No	No
σ	Medium	Highly	Highly	Highly	Medium	Highly	Highly	No

4.2 A Proposed Method

The selected macro parameters are elasticity modulus E, Poisson's ratio μ, and strength σ of the specimen. The selected micro parameters include: (1) physical parameters (e.g. density ρ, minimum radius $R_{\min}$ and ratio of maximum to minimum radius $R_{\max}/R_{\min}$); (2) mechanical parameters of grains (elasticity modulus E_P, stiffness ratio k_{nP}/k_{sP}, and friction coefficient μ_P); (3) mechanical parameters of parallel bonds (radius amplifier λ, elasticity modulus E_C, stiffness ratio k_{nC}/k_{sC}, average normal strength σ_C, standard deviation of normal strength S_{nC}, average tangential strength τ_C, and standard deviation of tangential strength S_{tC}).

Fundamental values of the selected micro parameters are proposed as follows:

(1) ρ: determined by actual values;
(2) $R_{\min}$: set to be 0.27 from Potyondy and Cundall [5];
(3) $R_{\max}/R_{\min}$: set to be 1.66 from Potyondy and Cundall [5];
(4) E_P: set to be $0.90E$, derived from 0.899 in Potyondy and Cundall [5];
(5) k_{nP}/k_{sP}: set to be 2.50, determined from Potyondy and Cundall [5];
(6) μ_P: set to be 0.50, determined from Potyondy and Cundall [5];
(7) λ: set as 1.00, determined from Potyondy and Cundall [5];
(8) E_C: set to be E_P, determined from Xu and Zhu [8];
(9) k_{nC}/k_{sC}: set to be k_{nP}/k_{sP}, determined from Xu and Zhu [8];
(10) σ_C: set to be 0.45σ (approximate to the average of 0.396 in Huang and Cen [3], 0.785 in Potyondy and Cundall [5] and 0.437 in Xia and Zhao [6]);
(11) S_{nC}: set to be $0.25\sigma_C$, determined from Xia and Zhao [6];
(12) τ_C: set to be 0.65σ (approximate to the average of 0.437 in Huang and Cen [3], 0.785 in Potyondy and Cundall [5], and 0.745 in Xia and Zhao [6]); and
(13) S_{tC}: set to be $0.25\tau_C$, determined from Xia and Zhao [6].

The number of the independent parameters is 3 (or, E_P, k_{nP}/k_{sP} and σ_C), coinciding with the number of the macro parameters (E, μ and σ), leading to the quick convergences in simulation. The evaluation of the simulation was justified by the summation of relative errors of each component of the macro parameters:

$$\begin{aligned}&\delta_1 = ((E - E^*)/E)^2, \delta_2 = ((\mu - \mu^*)/\mu)^2, \delta_3 = ((\sigma - \sigma^*)/\sigma)^2,\\&\delta = \delta_1 + \delta_2 + \delta_3\end{aligned} \tag{1}$$

Generally speaking, in the successive simulation steps, δ in (1) is monotonously increased or decreased. If the monotonously decrease occurred, the latter step would be performed using the corresponding decreased micro parameters with different times of those in the previous step. In the current study, the different times were defined as

$$M_{21} = M_{11}(1 + 2\delta_1), M_{22} = M_{12}(1 + 3\delta_2), M_{23} = M_{13}(1 + 4\delta_3) \tag{2}$$

where M_{21}, M_{22}, and M_{23} are the micro parameter magnitudes in the latter step corresponding to M_{11}, M_{12}, and M_{13} in the previous step, respectively to the maximum, medium, and minimum components (or δ_1, δ_2, and δ_3).

If the monotonously increase occurred, the micro parameters in the latter step will adjust using the equation

$$M_{21} = M_{11}(1 - 2\delta_1), M_{22} = M_{12}(1 - 3\delta_2), M_{23} = M_{13}(1 - 4\delta_3) \tag{3}$$

Then, the summation of the relatively errors δ will monotonously decreased. If the decreased δ reached to 0.02, the simulation would be ended. This was considered as the criterion of the simulation.

In a few of cases, the decreased δ does not reach to 0.02 and the increase in δ may occur in some later steps. In these cases, the micro parameters were considered as those used in the successive previous steps with the minimum components of the relatively errors.

4.3 Examples

Table 3 lists the examples in determining micro parameters using the above-mentioned techniques. In Table 3, actual distributions of compositions were considered in the example 1 for the Beishan granite; actual distributions of compositions were not considered in the example 2 for the Beishan granite; actual distributions of compositions were also not considered in the example 3 for the granite in Xia and Zhao [6].

From Table 3, it can be seen that convergence is much quick (only three steps) if the actual distributions considered; convergence is much slowly (six steps were used in the example 2) or not obviously convergent (example 3) if the actual distributions are not considered.

5 Summary

The video images photographed during uni-axial compression test were used to investigate the actual positions and types of the grains of granite. A micro model was developed in the two-dimensional particle flow code. Thirty-two orthogonal tests were then performed using seven micro mechanical parameters and four levels. The sensitivity analysis was also performed using the simulation results. A new method to determinate the micro mechanical parameters were proposed. It shows that the elasticity, Poisson's ratio and strength were much correlated between micro-macro scales; the convergence in particle flow simulations is much quick if the actual distributions are considered.

Table 3 Examples in determining micro parameters using macro parameters in particle flow simulation of granite

No.	Step	Independent micro parameters			Macro parameters in simulation			Micro parameters in simulation			Squared relative errors (1)			
		E_P/GPa	k_{nP}/k_{sP}	σ_C/MPa	E/GPa	μ	σ/MPa	E^*	μ^*	σ^*	δ_1	δ_2	δ_3	δ
1	1	2.64	2.500	16.68	2.93	0.149	37.1	3.33	0.22	24.56	0.019	0.210	0.110	0.340
	2	2.44	1.459	22.16				3.55	0.16	33.07	0.045	0.004	0.012	0.060
	3	2.22	1.438	22.94				3.27	0.16	36.74	0.013	0.006	0.000	0.019
2	1	2.64	2.500	16.68				3.33	0.22	22.65	0.019	0.202	0.151	0.372
	2	2.44	1.489	24.72				3.49	0.16	42.41	0.037	0.006	0.021	0.063
	3	2.26	1.456	23.18				3.38	0.16	37.44	0.024	0.005	0.000	0.028
	4	2.15	1.436	23.17				3.21	0.16	41.07	0.009	0.004	0.012	0.024
	5	2.09	1.415	22.63				3.00	0.17	30.27	0.001	0.012	0.034	0.046
	6	2.09	1.436	23.18				3.09	0.16	36.13	0.003	0.003	0.001	0.007
3	1	63.09	2.500	120.7	70.1	0.181	268.3	72.7	0.23	157.6	0.014	0.086	0.170	0.257
	2	62.74	1.857	161.8				82.4	0.20	261.3	0.031	0.014	0.002	0.045
	3	58.89	1.782	162.3				77.4	0.20	266.7	0.010	0.012	0.000	0.023
	4	57.04	1.739	162.3				75.9	0.20	251.6	0.007	0.010	0.004	0.021
	5	56.92	1.704	164.8				76.9	0.20	250.9	0.010	0.007	0.004	0.021
	6	55.85	1.669	167.6				74.2	0.19	236.8	0.004	0.005	0.014	0.022

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