A Rock Material Micro-Strength Calibration Model for Bonded Models in Particle Flow Code

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Abstract. Distinct Element Method (DEM) can accurately simulate the large deformation and crack propagation phenomenon of soft rocks. When employing the DEM method via Particle Flow Code, an initial issue is to calibrate the parameters utilized in the model. Typically, trial and error are used to achieve calibration; however, a lack of accuracy and time and effort requirements highly threaten its application. Based on the Parallel Bonded Model (PBM), we researched the bond’s failure criterion in this study. Then, the influence of micro parameters (tension strength $\sigma_c$ and cohesion strength $c$) on the rocks’ macro strength and failure mechanisms are studied. Two different test groups were considered by changing the two parameters (1): $c$ remains constant (2): $\sigma_c$ remains constant. The results illustrated that rock macro strength is positively correlated with its inferior PBM strength parameters. The macro strength will gradually stabilize at an upper boundary equal to $3.3c$ or $3.3\sigma_c$. With the increasing of $c$, the rock failure mechanisms vary from block fragmentation to shear failure. In general, the macro strength depends on the coupling effect of $c$ and $\sigma_c$ expressed with an exponential relationship. Through this relationship, only two steps are enough to calibrate the two micro-strength parameters. This research proposed a new way to calibrate PBM micro-strength parameters and provided insight into building the correlation between other micromechanical parameters in the DEM.

1. Introduction

The Distinct Element Method (DEM) can deal with discontinuous medium problems and analyze rock’s large deformation or crack propagation [1-4]. DEM has been widely applied in the simulation of rock mechanics [5], with the Particle Flow Code (PFC) being one of the most used tools [6]. However, it’s not mature to apply this method to largescale engineering problems. One of the problems is the low efficiency of calibrating the micro-strength parameters [7-8].

Calibrating parameters is the initial step in building a DEM model [9]. However, the traditional method, trial and error, is time-consuming and inaccurate [10]. Researchers have conducted several studies on micro parameters calibration. First, the influence of particle states on the mechanical...
properties is studied. Guo and Zhang et al. [11] studied the effect of particle shapes on mechanical properties by creating an anisotropic rock model with different clump components. Researches on particle size showed that the macro strength and elastic modulus are positively correlated with the ratio of model length to particle diameter [12-15]. The influence of contacting model’s parameters on macro mechanical properties was widely studied. Xu and Wu et al. [16] studied the effects of micro-strength parameters of the Bonded Model on rock’s tension strength by designing Brazilian tensile tests in DEM. Zhou and Xu et al. [17] proposed a systematic approach to calibrate the micro parameters for the Flat Jointed Model. Huang and Zhang et al. [18-19] studied the effects of micro parameters of the Smooth Joint Model on the macro mechanical properties. Xia and Zhao et al. [20] investigated the relationship between the Clump Bonded Model’s micro and macro mechanical parameters. In addition, many researchers focused on the properties of the Parallel Bonded Model (PBM). These works have revealed that the model’s peak strength is affected mainly by micro cohesion strength \( c \) when the ratio of \( c \) to tension strength \( \sigma_c \) is less than 2 [21-24]. However, these research results only show the qualitative effects of \( c \) and \( \sigma_c \). Lots of “trial and error” work are also required when calibrating those micro parameters.

Hence, we designed an orthogonal DEM simulation test for the PBM to efficiently calibrate micro-strength parameters when building DEM models. In addition, we have studied the relationship between micro parameters and macro strength. Two kinds of tests were conducted: (1): \( c \) remains constant (2): \( \sigma_c \) remains constant.

2. Methods and contents

2.1. Parallel Bonded Model (PBM)

Figure 1 shows the components of PBM, from which we can find that some bonds are acting on the contacts between the particles. These bonds can resist tension and shear forces. The specific physical models are shown in figure 1. PBM involves two states (unbonded and bonded), indicating linear elastic property in the unbonded state.

![Figure 1. The illustration of PBM.](image)

Applying PBM is similar to the process of bonding the particles with cement which resembles a rock material. PBM can be regarded as a combination of two pairs of parallel springs with normal and tangential stiffness. However, the bonded parts can be destroyed under ultimate load, and the failure criterion is shown in figure 2. Note that there is no specific constitutive relation in the DEM system. To meet the needs of researchers, we need to calibrate many micro parameters of DEM particles and bonds. Typically, this process is accomplished by a trial and error process, which is time-consuming. Because the strength is critical to the simulation results, we mainly focused on the micro-strength parameters.
Yet, the model’s failure is even closely related to the bonds damage. Therefore, it’s essential to figure out the criterion of bonds failure in the simulation process.

![Figure 2. Strength envelope of bonds.](image)

The bonds can be damaged when subjected to tension or shear forces. The calculating process in PFC is shown as following:

1. Updating the basic physical parameters:
   \[
   R = \min(R^1, R^2) \\
   A = 2Rt (t = 1) \\
   I = \left(\frac{2}{3}\right)R^3t
   \]
   (1) (2) (3)

   The model will compute a minimum \( R \) by equation (1) and calculate it in equations (2) and (3), where \( A \) is the area of bonding section and \( I \) is the moment of inertia.

2. Updating the normal force:
   \[
   F_n = F_n + k_n A \Delta \delta_n
   \]
   (4)
   Where \( \Delta \delta_n \) is normal displacement and \( F_n \) is normal force and the \( k_n \) is the normal stiffness.

3. Updating shear force \( F_s \):
   \[
   F_s = F_s - k_s A \Delta \delta_s
   \]
   (5)
   Where \( \Delta \delta_s \) is shear displacement and \( k_s \) is the tangential stiffness.

4. Updating bending moment \( M_b \) in the cross-section:
   \[
   M_b = M_b - k_n I \Delta \theta_b
   \]
   (6)
   Where \( \Delta \theta_b \) is bending angle increment.

5. Updating the normal stress and tangential stress:
   \[
   \sigma = \frac{F_n}{A} + \beta \frac{M_b R}{I} \\
   \tau = \frac{F_s}{A}
   \]
   (7) (8)

   In this step, the normal and tangential stresses can be calculated using equations (7) and (8).

6. Determining bond breakage according to the criterion shown in figure 2:
   In this step, the code will ascertain whether the bonds will be broken under tension forces. Then, the tangential shear force will also be compared with the formula \( \tau = c - \sigma \tan \varphi \).

The abovementioned steps are used for the damaging bond criterion, which is initial to the failure of the DEM model. The bonds failure process is closely related to the parameters of \( c \) and \( \sigma_c \). However, there are more than two parameters in the DEM. Beside \( c \) and \( \sigma_c \), the other parameters such as stiffness, friction angle, particle size, model size, etc., are also crucial to the mechanical behavior of the DEM rock models. Therefore, in the next section, the specific assignment of those parameters is discussed.

2.2. The schemes of DEM simulation experiments

In this section, we explained the schemes of the experiments and gave the specific parameters.
A DEM model is composed of many particles and bonds with many associated parameters. The ratio of the normal stiffness $k_n$ to tangential stiffness $k_s$ influences the crack propagation and failure mode but has little effect on the macro strength [20]. In scale effect, the influence of particle size on macro strength is low if the ratio of the model’s length to particle radius is large than 50 [12]. The friction coefficient affects the mechanical properties of sand-like materials, but it has minimal effects on the rock models. In general, only $c$ and $\sigma_c$ influence the macro strength, which can also be explained by the bonds failure criterion in section 2.1. Therefore, in this study, we mainly investigated the influence of cohesion $c$ and tension strength $\sigma_c$ on the macro strength.

![Graph showing stress-strain curves for simulation and experiment results.](image)

**Figure 3.** Calibration results with experiments.

This study focused on soft rock engineering, with the given basic parameters based on experimental results of the typical soft rocks in southern China. The experiments were carried out in a previous study [25], and the calibrating result is shown in figure 3. Figure 3 (a) shows the stress-strain curves of simulation and experimental results. Except for the strain error in the compaction stage, this calibrating process is consistent with soft rock’s mechanical behavior. In addition, figure 3 (b) shows the cracks results of simulation and experiments, with the main crack’s direction being similar. Finally, table 1 shows the calibration details.

**Table 1.** The particle and bonds parameters in DEM model of this paper.

| Parameter      | Value        | Notes                  |
|---------------|--------------|------------------------|
| $R$ (m)       | $3 \times 10^{-5} - 5 \times 10^{-5}$ | Radius                 |
| $\rho$ (kg/m$^3$) | 2500         | Density                |
| Porosity      | 0.1          | Porosity               |
| $k_n$ (N/m)   | $5 \times 10^9$ | Normal stiffness       |
| $k_s$ (N/m)   | $5 \times 10^9$ | Shear stiffness        |
| $\mu$ (°)     | 30           | Friction angle         |
| $F$           | 0.57         | Friction coefficient   |
| $g_r$ (m)     | $5 \times 10^{-6}$ | Bond gap              |
| $E^*$ (GPa)   | 0.5          | Effective modulus      |
| $k^*$         | 2.0          | Ratio of normal to shear stiffness |
| $\beta$       | 0.5          | critical damping ratio |
| damp          | 0.7          | Ball local damping coefficient |
| $\bar{k}_n$ (N/m) | $5 \times 10^9$ | Normal stiffness of bonds |
| $\bar{k}_s$ (N/m) | $5 \times 10^9$ | Shear stiffness of bonds |
In section 2.1, we studied the failure process of bonds and have found that the bonds’ strength depends on $c$ and $\sigma_c$. Therefore, it is necessary to design orthogonal tests to study the effects of $c$ and $\sigma_c$ on the macro-strength.

The orthogonal tests are carried out based on the parameters in Table 1. Figure 4 shows the experimental scheme, note that the value of $c$ in the fixed $\sigma_c$ tests varied from 0 to about 3.3 $\sigma_c$ and the value of $\sigma_c$ in the fixed $c$ tests also varied from 0 to about 3.3 $c$.

2.3. The proposing of the calibration model.

According to the failure criterion of PBM, we know that the bonds may fail under tension or shear xy. Generally, when a load is applied, two kinds of forces co-exist in the sample. Therefore, the value of $c$ and $\sigma_c$ will yield a coupling effect on the final strength, and the smaller one will restrict the macro-strength. We have done a lot of work on obtaining a relation to describe the coupling effect of $c$ and $\sigma_c$.

The variate is controlled between $c$ and $\sigma_c$ in this paper according to the experimental schemes shown in Figure 4. We increased $c$ under a constant $\sigma_c$ in the first group of experiments, where the values of $\sigma_c$ are 5 MPa, 10 MPa, 15MPa, 20MPa, respectively. Similarly, we executed the simulation tests by increasing the value of $\sigma_c$ under a fixed value of $c$ in another group of experiments. Series of strength were obtained. We found that the sample’s peak strength increased rapidly during the early stage and gradually vanished to 0 in the experiments. There is a coupling effect between $\sigma_c$ and $c$; when the ratio of $c/\sigma_c$ is less than 2, the macro strength is affected mainly by $c$ and when the ratio of $c/\sigma_c$ is greater than 2, the value of $\sigma_c$ will restrict the final macro strength.
We can use an exponential relation (9) to describe the abovementioned coupling effect, where \( y(\sigma, c) \) represents the macro peak strength of the sample and \( k \) is the shape parameter for the relation. In the following sections, we will use the sign of \( \sigma \) to replace the \( \sigma_c \) for simplicity.

\[
y(\sigma, c) = A(c) \cdot e^{\left(-\frac{\sigma}{kc}\right)} + B(c)
\]  

(9)

When \( \sigma \) is the variate, the partial differential equation (10) shows the law of strength evolution, and we can easily find the \( y' \) tends to 0 when \( \sigma \) tends to infinity.

\[
y' = -\frac{A(c)}{kc} \cdot e^{\left(-\frac{\sigma}{kc}\right)}
\]  

(10)

When \( c \) is the variate, the partial differential equation (11) shows the law of strength evolution too. When \( c \) tends to infinity, the equation (11) can be simplified to

\[
y' = A'(c) \cdot e^{\left(-\frac{\sigma}{kc}\right)} + A(c) \cdot \left[e^{\left(-\frac{\sigma}{kc}\right)} \cdot \left(\frac{\sigma}{kc}\right)^2\right] + B'(c)
\]  

(11)

In the next section, we will show the performance of this exponential relation based on the results of orthogonal test results, along with some verifications.

3. Results and discussion

3.1. Experimental results of fixing \( c \).

Figure 5 shows the crack formats of the DEM model when \( c \) is 10 MPa. The crack propagation formats vary with the increase in \( \sigma_c \). When \( \sigma_c \) is less than 5 MPa, many fully developed wing cracks were observed in the failure state. On the contrary, when \( \sigma_c \) is greater than 5 MPa, only one main crack with a few wing cracks is seen in the final state. This phenomenon is caused by the coupling effect of \( c \) and \( \sigma_c \). When \( \sigma_c \) is much smaller than \( c \), even a small tension force will damage the bonds and produce many wing cracks. Therefore, the impact of \( c \) will be restricted in the failure process.

Figure 6 shows the macro strengths from the simulations. The curves show a similar increasing trend. When \( c \) remains constant, the macro-strength increased rapidly and then decreased until it became constant. We can easily fit those macro strengths by equation (9), and the results are shown in equations (12), (13), (14), (15), respectively.

\[
c = 5\text{MPa}:
\]

\[
y = -19.08 \exp\left(-\frac{\sigma}{3.19}\right) + 17.86
\]

(12)

\[
c = 10\text{MPa}:
\]

\[
y = -34.85 \exp\left(-\frac{\sigma}{6.43}\right) + 33.38
\]

(13)

\[
c = 15\text{MPa}:
\]

\[
y = -51.50 \exp\left(-\frac{\sigma}{9.58}\right) + 49.25
\]

(14)

\[
c = 20\text{MPa}:
\]

\[
y = -67.72 \exp\left(-\frac{\sigma}{13.20}\right) + 66.47
\]

(15)

Table 2. Calculated parameters in equation 9.

| \(c/\text{MPa} \) | \(-A(c)\) | \(B(c)\) | \(k_c\) | \(-A/c\) | \(-A/B\) | \(B/c\) | \(k\) |
|-----------------|-----------|--------|--------|----------|----------|----------|-----|
| 5               | 19.08     | 17.86  | 3.19   | 3.816    | 1.068    | 3.572    | 0.638|
| 10              | 34.85     | 33.38  | 6.43   | 3.485    | 1.044    | 3.338    | 0.643|
| 15              | 51.50     | 49.25  | 9.58   | 3.433    | 1.045    | 3.283    | 0.638|
| 20              | 67.72     | 65.58  | 13.20  | 3.386    | 1.032    | 3.279    | 0.660|
| average         | 3.53      | 1.047  | 3.368  | 0.644    |          |          |      |
Figure 5. Parts of results when \( c = 10 \) MPa.

\[
y = -67.72 \exp(-\sigma_c/13.20) + 66.47
\]

\[
y = -51.50 \exp(-\sigma_c/9.58) + 49.25
\]

\[
y = -34.85 \exp(-\sigma_c/6.43) + 33.38
\]

\[
y = -19.08 \exp(-\sigma_c/3.19) + 17.86
\]

Figure 6. Test experimental results of fixing \( c \).
The obtained parameters are shown in table 2. Therefore, we can derive the following relation: \( A(c) = -3.53c, B(c) = 3.368c, k = 0.644 \). Then, a specific calibration relation of \( c \) and \( \sigma_c \) is obtained:

\[
y = -3.53c \exp\left(-\frac{\sigma}{0.644c}\right) + 3.368c
\]

(16)

3.2. Experimental results of fixing \( \sigma_c \).

Figure 7. Parts of results when \( \sigma_c = 10 \text{ MPa} \).

Figure 7 shows the crack formats of the DEM model when \( \sigma_c \) is 10 MPa, similar to the results of fixing \( c \). We can find that the crack propagation formats vary with increasing \( c \). When \( c \) is less than 4 MPa, many fully developed wing cracks are observed in the failure state. On the contrary, when \( c \) is greater than 4 MPa, one main crack with a few wing cracks is shown in the failure mode. This phenomenon is also caused by the coupling effect of \( c \) and \( \sigma_c \). When \( c \) is much smaller than \( \sigma_c \), even a small shear force will damage the bonds and produce many wing cracks. Therefore, the effect of \( \sigma_c \) will be limited in the failure process.

In section 2.3, we provided the relation (11) to describe the variation law of macro strength with the changing of \( c \), which is more complicated than relation (10). This phenomenon can be found in figure 8. Figure 8 shows the test results when \( \sigma_c \) remains constant. Those curves show similar trends. When \( c \) increases, the strengths of samples firstly increase linearly, and then stabilize at a final value. However, these curves are not smooth, and it’s hard to give a relation when the variate is \( c \).
As shown in figure 8, those curves finally stabilize at upper boundaries, which are limited by the $\sigma_c$. The strength data is positively correlated with the value of $c$ before those critical points. We can obtain these critical points from figure 8. The ratio value of $c/\sigma_c$ in the four critical points is 2.2, 1.9, 1.87, 1.8, respectively. These values are close to 2, similar to the conclusions derived by other researchers [21-24]. It is believed that the macro-strength is mainly affected by $c$ when $c/\sigma_c$ is less than 2, and the macro-strength is mainly controlled by $\sigma_c$ when $c/\sigma_c$ is greater than 2. Therefore, in combination with equation (11), the following expression can be derived:

$$y' = \begin{cases} A'(c) \exp\left(-\frac{\sigma}{kc}\right) + A(c) \left[\exp\left(-\frac{\sigma}{kc}\right) \left(\frac{\sigma}{kc^2}\right)\right] + B'(c); & 0 < \frac{\sigma}{c} < 2 \\ A'(c) + B'(c); & 2 < \frac{\sigma}{c} \end{cases}$$

(17)

In addition, the value of $A'(c) + B'(c)$ equals to 0 according to the equation (16), which is consistent with the curves shown in figure 8.

According to the strength results, the values of $\sigma_n/\sigma_c$ at the critical points were derived, and the average value is 3.3, which reveals the value of upper boundary. We can also get a similar result by analyzing the ultimate strength in figure 6, and it is expressed as $\sigma_n=3.3c$. Therefore, when applying PBM in DEM, the ultimate macro-strength of models will be restricted at $3.3\sigma_c$ or $3.3c$.

3.3. Discussion

| Table 3. The verification of calibration relation. |
|-----------------------------------------------|
| c/MPa | $\sigma_c$/MPa | $\sigma_n$ results of simulations/MPa | $\sigma_n$ calculated by relation/ MPa | error/MPa | ratio of error/% |
|-------|----------------|--------------------------------------|--------------------------------------|-----------|-----------------|
| 1     | 11             | 5                                    | 16.8                                 | 17.8      | 1               | 5.9%            |
| 2     | 10             | 19                                   | 33.8                                 | 34.4      | 0.6             | 1.8%            |
| 3     | 15             | 28                                   | 49.6                                 | 51.3      | 1.7             | 3.4%            |
| 4     | 20             | 36                                   | 63.6                                 | 67.6      | 4               | 6.2%            |

We derived the calibration relation (16) when the variate is $\sigma_c$. If we apply the specific $c$ and $\sigma_c$ to equation (16), the strength can be calculated. Therefore, we can verify the feasibility of this equation by the results of fixing $\sigma_c$ in section 3.2. We have selected the four critical points in figure 8 to verify the calibration relation in this study. Table 3 shows the strength error calculated by the equation (16), which are 5.9%, 1.8%, 3.4%, and 6.2%, respectively. The average error is 4.3%; hence the calibration relation given in equation (16) can be considered reliable within the error of 5%.
According to equation (16), to calibrate the model’s strength, we only need to pick the specific micro-strength parameters in 2 steps (see figure 8). Therefore, using the exponential relation proposed in this study allows us to conveniently and effectively calibrate the micro-strength parameters in two steps instead of trial and error.

4. Conclusions

- The exponential relation proposed in this study can well describe the coupling effect of $\sigma_c$ and $c$, the error between the calibration results and the target strength is less than 5%, which can be applied to calibrate rock and soil materials.
- In this study, the influence of the micro-strength parameters on the macro-strength and deformation is studied through groups of orthogonal experiments. The upper boundary macro-strength of the two experiments can be expressed as $3.3c$ or $3.3\sigma_c$.
- Using the exponential mathematical model to establish relationships between DEM strength parameters provides insight into dealing with other micro parameters.

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