Bonded-particle model calibration using response surface methodology

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A B S T R A C T
The bonded-particle model (BPM) is commonly used in numerical analysis of the mechanical behavior of rock samples. Constructing a BPM model requires specification of a number of microstructural parameters, including the parallel-bond tensile strength, parallel-bond cohesion strength, parallel-bond effective modulus, parallel-bond friction angle, and parallel-bond stiffness ratio. These parameters cannot be easily measured in the laboratory or directly related to either measurable or physical material parameters. Hence, a calibration process is required to choose the values to be used in simulations of physical systems. In this study, response surface methodology along with the central composite design approach is used to calibrate BPMs. The sensitivities of the microparameters related to the uniaxial compressive strength (UCS) and elasticity modulus (i.e., the macroscopic responses of the models) are thoroughly scrutinized. Numerical simulations are performed to carefully assess the performance of the model. It is found that the elasticity modulus is highly correlated with the parallel-bond effective modulus. In addition, the parallel-bond tensile and cohesion strengths are the two most significant microparameters with a considerable effect on the UCS. The predicted values determined by the proposed approach are in good agreement with the observed values, which verifies the applicability of the proposed method.

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Introduction

The discrete element method (DEM) or so-called distinct element method is regarded as an effective approach for engineering problems in granular and discontinuous materials. It has been widely used for granular flows, powder mechanics, rock mechanics, and comminution (Zhang, 2010). In addition, this method has been extensively used to simulate tumbling mills (Cleary, 1998; Cleary, Morrison, & Morrell, 2003; Delaney, Cleary, Morrison, Cummins, & Loveday, 2013; Djordjevic, 2005; Khanal & Jayasundara, 2014; Mishra & Rajamani, 1992; Powell, Weerasekara, Cole, LaRoche, & Favier, 2011; Rajamani, Songfack, & Mishra, 2000; Wang, Yang, & Yu, 2012) and stirred mills (Plochberger & Avila, 2014; Sinnott, Cleary, & Morrison, 2006). A recent study has also verified the application of the DEM to comminution science (Cleary & Sinnott, 2015; Weerasekara et al., 2013).

The DEM is used to solve Newton’s equations of motion, based on which particle motion can be effectively handled. Based on the contact law, the forces in interparticle contact can be determined (Weerasekara et al., 2013). Classical DEM simulations do not involve particle breakage, and hence they are most suitable for simulation studies of flow in non-breakable materials. This approach can also be applied to flows where the intensity of breakage can be determined from the energy spectrum. However, in some cases, such as the crushing chamber of crushers, it is essential to simulate the actual size reduction of particles in the flow of granular material. Because particles tend to move down in the crushing chamber, their size has to be reduced according to the applied forces (Herbst & Potapov, 2004). In the literature, there has been little tendency to simulate the crushing machine. This is mainly because of the following points: (a) to allow the particles to pass through the equipment, it is necessary to directly include breakage in the simulations, (b) it increases the number of particles in the crusher and thus results in a larger model size, and (c) it results to a high level of geometric complexity in the crusher (Cleary & Sinnott, 2015).

Different methods are used to model rock material breakage in the DEM. The population balance replacement model is the most commonly used approach. In this approach, if a load constraint is exceeded, a particle is replaced by a set of progeny particles. The size distribution of these particles is calibrated based on the breakage

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test data (Quist & Evertsson, 2016). Potyondy and Cundall (2004) proposed the bonded-particle model (BPM). This approach uses imaginary beams among the contacted particles to bond a cluster of subparticles. A third approach applies tetrahedral mesh elements to model a specific particle. In this approach, compliant contacts and stress constraints are considered in both the normal and tensile directions.

A recent report by Lisjak and Grasselli (2014) provides a complete review of the different approaches used to model breaking of rock particles. For instance, Herbst and Potapov (2004) and Quist and Evertsson (2010) focused on developing models for lab-scale cone crushers. Single particle breakage in jaw crushers was investigated by Refahi, Mohandes, and Rezai (2010). It should be mentioned that all of the mentioned approaches are based on BPMs. A method has been developed to model discrete grain breakage (Herbst & Potapov, 2004). The method treats the crusher based on a bonded sphere model including bonded tetrahedral elements. Lichter, Lim, Potapov, and Kaja (2009) introduced the fast breakage model. This approach uses polygonal elements to include DEM particles. Following a fracture event, particle replacement of the breakage progeny is realized based on a macroscale population balance model (Lisjak & Grasselli, 2014).

The BPM has been used to investigate the mechanical behavior of rocks (Cundall & Strack, 1979; Ivars et al., 2011; Kulattikale, Malama, & Wang, 2001; Potyondy & Cundall, 2004) and characterize the breakage properties of rocks in milling or crushing (Refahi et al., 2010; Whittles, Kingman, Lowndes, & Jackson, 2006). The same approach was also used to investigate rail ballast (Thakur, Vinod, & Indraratna, 2010), where the authors used the particle-flow code in two-dimensions with simple breakage models. Using a similar approach, Estay and Chiang (2013) proposed application of the particle-flow code in three-dimensions. It is well-known that each collection of grains that is joined by cement shows specific mechanical behavior. The BPM replicates such behavior in rock (Weerasekara et al., 2013). Similar approaches, such as the Rumpf model (Laitinen, Bauer, Niinimäki, & Peuker, 2013; Rumpf, 1990; Sigmund, El-Shall, Shah, & Moudgil, 2008), are available in other research fields. These models can also include structural properties such as the bond strength and bond cross-sectional area to represent the aggregate strength.

The basic concept of the traditional BPM is to represent the rock as densely packed disks or spheres that are bonded together at their contacts, and then simulate its mechanical behavior. If an adequate control action is performed on the strength and mechanical properties of the bonds, it results in similar behavior to that of the mechanical properties of the rock material (Weerasekara et al., 2013). The mechanical behavior of a BPM specimen is described by the movement of each particle along with the forces and moments acting at each contact between two constitutive particles (Ding & Zhang, 2014). The bond is represented by a thin finite area plate (Fig. 1(a)) and includes five parameters: the normal and shear stiffnesses per unit area $k_n$ and $k_s$, the tensile and shear strengths $\sigma_t$ and $\tau_t$, and the bond-radius multiplier, $\tau$, which defines the bond radius $R = \tau \min(R_n, R_s)$, with $R_n$ and $R_s$ being the radii of the bonded particles. The relative motions between the two contact particles cause changes in the contact forces and moments owing to the contact stiffness. The forces and moments acting at the contact are shown in Fig. 1(b).

The particle movements and the resultant forces and moments follow Newton's law of motion. The change of the contact forces and moments owing to the relative particle movement are determined by

$$\Delta F_n = -k_n A \Delta d_n, \quad \Delta F_s = -k_s A \Delta d_s,$$  \hspace{1cm} (1)

$$\Delta \tau_n = -k_n \Delta \theta_n, \quad \Delta \tau_s = -k_s \Delta \theta_s,$$  \hspace{1cm} (2)

where $F_n$, $F_s$, and $\tau_n$, $\tau_s$ are the contact forces and moments at the center of the contact zone, respectively, in the normal ($n$) and shear ($s$) directions, $d_n$, $d_s$ and $\theta_n$, $\theta_s$ are the relative displacements and rotations between the two bonded particles, respectively, in the normal ($n$) and shear ($s$) directions; and $A$, $I$, and $J$ are the area, moment of inertia, and polar moment of inertia of the bond cross-section, determined by (Ding & Zhang, 2014; Potyondy & Cundall, 2004)

$$A = \pi R^2, \quad I = \frac{1}{4} \pi R^4, \quad J = \frac{1}{2} \pi R^4.$$  \hspace{1cm} (3)

The maximum tensile and shear stresses, $\sigma_{\text{max}}$ and $\tau_{\text{max}}$, acting at the contact are obtained by (Ding & Zhang, 2014)

$$\sigma_{\text{max}} = \frac{F_n}{A} + \frac{M_n}{I},$$  \hspace{1cm} (4)

$$\tau_{\text{max}} = \frac{F_s}{A} + \frac{M_s}{J}.$$  \hspace{1cm} (5)

If $\sigma_{\text{max}} \geq \sigma_t$ or $\tau_{\text{max}} \geq \tau_t$, the bond breaks by tension or shear and the bond along with its forces, moments, and stiffness is then removed from the particle (Ding & Zhang, 2014).

In DEM analysis, it is crucial to select appropriate parameters for accurate simulation of real and physical systems (Hanley, O’Sullivan, Oliveira, Cronin, & Byrne, 2011). For numerical simulations using DEM implemented in the particle-flow code (PFC), the macroscale mechanical properties of the rock cannot be directly included in the model. Only macroscale mechanical parameters are specified for the particle assembly that hypothetically represents the actual rock material (Wang, Xu, Li, Liu, & Peng, 2013). A higher confidence degree is attained in estimating/measuring the input parameters, namely, the particle dimensions or their density. However, experimental studies fail to identify the rheological parameters as inputs for contact constitutive models (Hanley et al., 2011). Therefore, a calibration approach is often used to select these parameters. Typically, calibration involves varying the DEM parameters until the model response closely corresponds to the equivalent physical experimental response. While conceptually simple, this calibration approach has many drawbacks: it may take several trial tests and a long time to obtain an appropriate set of parameters, it is impossible to know how many DEM simulations are required for calibration in advance, the final parameters obtained may not be optimal, and the mechanistic insight gained is limited (Hanley et al., 2011).

In the calibration process, two main steps need to be performed. The first step is parameter identification (Wang & Tonon, 2009), which relates the microparameters to the macromaterial properties. The second step is called parameter quantification, which assigns the parameters certain values to reproduce the experimental behavior of the testing material. Parameter identification of the BPM has been discussed by Potyondy and Cundall (2004). The framework of this method is shown in Fig. 2. Uniaxial compression tests are simulated and then compared (steps 1 and 2). Hsieh, Li, Huang, and Jeng (2008) proposed a similar concept, where uniaxial compression is firstly modeled using the BPM and it is iteratively revised until it gives reasonable macroscopic uniaxial compression behavior (similar uniaxial compressive strength (UCS) and Young’s modulus). This test also determines the BPM microscopic parameters (Hsieh et al., 2008). The only approach to allocate the microparameters of the PFC model is the “trial and error” method. However, it is a primitive method aligned with a high computational burden. Only a few attempts have been made to improve and
simplify the calibration procedure (Hsieh et al., 2008; Potyondy & Cundall, 2004).

Only a limited number of researchers have focused on developing methods for parameter quantification. Most of the studies using the DEM give the parameters used for the materials without mentioning the calibration process. It has been found that the trial and error approach is commonly used with the corresponding limitations (Zhang, 2010). Recently, there have been some attempts to develop more efficient DEM calibration approaches using design of experiments (DOE) methods (Hanley et al., 2011). DOE is defined as a structured and organized method for determining the relationship between the factors affecting a process and the output of that process (Yoon, 2007). There are many different DOE methods, and the best choice depends on the objectives of the analysis and the number of factors to be investigated. Table 1 gives the details of DOE methods categorized by the experimental objectives that they meet. Yoon (2007) applied a Plackett–Burman design and response surface analysis to determine suitable DEM microparameters for uniaxial compression of bonded rock particles. Favier, Curry, and LaRoche (2010) used DOE methods to calibrate DEMs for a mixer and a hopper based on measurements of the torque and discharge flow rate, respectively. Johnstone and Ooi (2010) applied DOE methods to find appropriate model parameters based on experimental measurements of the flow in a rotating drum device and the mechanical response during a confined compression test (Hanley et al., 2011).

In this study, we used response surface methodology (RSM) to both identify and quantify the important micromechanical parameters. The established approach also considers the possible interactions between the micromechanical parameters in BPM calibration. Central composite design (CCD) was chosen as the design matrix because it allows reliable identification of the first-order interaction between the factors and provides a second-order polynomial model to predict the optimum levels of these parameters (Montgomery, 2008). By modeling and optimizing the parameters, it was possible to investigate the effects of the independent

![Fig 1. Contact model, for (a) the bond between two particles, and (b) the forces and moments acting on the bond (Müller & Tomas, 2014).](image1)

![Fig 2. Schematic illustration of the framework of conventional BPM calibration (Hsieh et al., 2008).](image2)
parameters on the dependent parameters, i.e., the UCS and the elasticity modulus ($E$). The independent parameters included the parallel-bond effective modulus, ratio of the parallel-bond normal to the shear stiffnesses, parallel-bond tensile strength, parallel-bond cohesion strength, and parallel-bond friction angle. Extensive numerical simulations were performed to investigate the effectiveness of the proposed approach. The obtained results are discussed in detail.

**Materials and methods**

**Rock specimen**

The mechanical properties (UCS and elasticity modulus) of natural limestone obtained from the Gheshlagh quarry in Iran were experimentally evaluated. Standard compression tests were performed on ten cylindrical specimens with a diameter of 54 mm and a height of 135 mm. To estimate the dry density of the limestone based on the saturation and caliper technique, the standards of International Society for Rock Mechanics were strictly followed. The mechanical properties of the studied rocks are shown in Table 2 (Refahi et al., 2010).

**Numerical modeling of the UCS test**

Three-dimensional simulations of the UCS test were performed using the Particle Flow Code in three Dimensions (PFC3D) based on the DEM which was provided by Itasca Consulting Group, Inc. in USA. This software package is an industrial implementation of the DEM algorithm proposed by Cundall and Strack (1979). A DEM synthetic cylindrical model of the rock sample with a diameter of 50 mm and a height of 100 mm was created to simulate the experimental UCS test, as shown in Fig. 3. The model consists of 9594 spherical particles with randomly distributed radii ranging from 1.0 to 2.0 mm. A process analogous to physical compaction was used for sample preparation and the sample packed in a way to approach the actual rock properties (porosity 0.2 and bulk density 2090 kg/m$^3$). The testing conditions assume that the top and bottom plates behave as rigid bodies with zero contact friction.

**Design of experiment**

**Response surface methodology**

RSM is a collection of statistical and mathematical methods for modeling and analyzing engineering problems. In this technique, the principle goal is to optimize the response surface influenced by diverse process parameters. RSM determines the relationship between the controllable input parameters and the obtained response surfaces (Kwak, 2005). The design procedure for RSM is as follows (Gunaraj & Murugan, 1999):

(i) Design a series of experiments for sufficient and reliable measurement of the desirable response.

(ii) Develop a mathematical model with a second-order response surface and maximum fitting.

(iii) Determine the most desirable set of experimental parameters that produce a maximum or minimum value of the response.

(iv) Express the direct and interactive effects of the process parameters as two- and three-dimensional plots.

In the case where all of the running variables are measurable, the response surface can be expressed as

$$y = f(x_1, x_2, x_3, \ldots, x_n),$$

where $y$ is the response of the system and $x_i$ are the variables of action (called factors). The objective is to optimize the response variable ($y$). It is assumed that the independent variables are continuous and controllable by experiments with negligible errors. In addition, establishing a correct approximation for the true functional relationship between the independent variables and the response surface is required (Gunaraj & Murugan, 1999).

**Central composite design**

The experimental design methods that are commonly used for process modeling and analysis are mainly categorized as full-factorial, partial-factorial, and central composite design approaches. For full-factorial design, at least three levels per variable are required to estimate the coefficients of the quadratic terms in the response model. Therefore, concerning the three independent process variables mentioned in Section Introduction, a number of experiments as well as replications should be performed (Box & Wilson, 1951). It is obvious that partial-factorial design
requires fewer experiments than full-factorial design. Nevertheless, the former is useful if certain variables are already known to show no interaction (Box & Hunter, 1961; Obeng, Morrell, & Napier-Munn, 2005). An efficient alternative to factorial design is CCD, which was originally developed by Box and Wilson (1951) and then improved by Box and Hunter (1957). CCD gives nearly as much information as three-level factorial design and needs fewer tests than full-factorial design. It has also been shown to be adequate to describe the majority of steady-state process responses (Gilliers, Austin, & Tucker, 1992). The number of tests required for CCD involves the standard $2^k$ factorial with its origin at the center, 2k points fixed axially at a distance, e.g., $\alpha$ from the center to generate the quadratic terms, and replicate tests at the center, where $k$ is the number of variables. The axial points are chosen so that they make rotation possible (Box & Hunter, 1957), which guarantees that the variance of the model prediction is constant at all points equally distant from the design center. Replicates of the test at the center are very important because they provide an independent estimation of the experimental error. For five variables, six tests at the center are suggested (Box & Hunter, 1957). Consequently, the total number of tests necessary for five independent variables in the half replicate of CCD is $2^{(5-1)} + (2 \times 5) + 6 = 32$ (Box & Hunter, 1957; Obeng et al., 2005). After defining the desired ranges of values for the variables, they are coded to lie at ±1 for the factorial points including 0 for the center points and ±$\alpha$ for the axial points. As shown in Table 3, the codes are calculated as functions of the desirable range for each factor (Aghaie, Pazouki, Hosseini, Ranjbar, & Ghavipanjeh, 2009).

By obtaining the response data from the test work, a regression analysis technique is performed to determine the coefficients of the response model, namely, ($b_1, b_2, \ldots, b_n$), their standard errors, and their significance. In addition to constant ($b_0$) and error ($\varepsilon$) terms, the response model incorporates the following items (Obeng et al., 2005):

- Linear terms in each variable ($x_1, x_2, \ldots, x_n$);
- Squared terms in each variable ($x_1^2, x_2^2, \ldots, x_n^2$);
- First-order interaction terms for each paired combination ($x_1 x_2, x_1 x_3, \ldots, x_{n-1} x_n$).

Therefore, for the three variables under consideration, the response model is

$$y = (b_0 + \varepsilon) + \sum_{i=1}^{5} b_ix_i + \sum_{i=1}^{5} b_{i2}x_i^2 + \sum_{i=1}^{5} \sum_{j=i+1}^{5} b_{ij}x_ix_j.$$  

(7)

The $b$ coefficients, which should be determined in the second-order model, are obtained by the least squares method. In general, Eq. (7) can be written in matrix form:

$$Y = bX + \varepsilon,$$  

(8)

where $Y$ is a matrix of measured values and $X$ is a matrix of independent variables. The matrices $b$ and $\varepsilon$ consist of coefficients and errors, respectively. The solution to Eq. (8) can be obtained by the matrix approach (Gunaraj & Murugan, 1999; Kwak, 2005).

$$b = (X^TX)^{-1}X^TY.$$  

(9)

where $X^T$ is the transpose of matrix $X$ and $(X^T)^{-1}$ is the inverse of matrix $X^TX$.

The coefficients, namely, the main effect ($b_i$) and two-factor interactions ($b_{ij}$), can be estimated from the experimental results by applying the least squares method using Design Expert 7 Trial
(State Ease, Inc., Minneapolis, MN, USA). To determine the significance of each term in the equation and estimate the goodness or fitting quality, the polynomial equation for the response is validated by analysis of variance (ANOVA) (Ferella, De Michelis, Scocchera, Pelino, & Vegliò, 2015).

### Experimental design

Half replicate CCD was chosen to design a series of experiments to provide suitable data to determine the relationship between the response (i.e., the UCS and elasticity modulus) and the five microparameters. Considering the relationships in Table 3, the corresponding actual levels are given in Table 4.

With five factors, the total number of possible combinations with three main levels is $3^5 = 243$. Hence, inspecting this solution space with only 32 simulations obtained from half replicate CCD remains a very efficient approach. Table 5 summarizes the parameters and levels used for each of the 32 test runs along with their results and predicted output values.

The calibrated parameters are determined by matching the calculated macroscopic strength (UCS) and elasticity modulus (E) with the experimentally measured values listed in Table 2. The model parameters are determined based on a curve-fitting approach, and the running variables are listed in Table 5. Fig. 4 compares the stress–strain curves obtained by experiments and the calibrated numerical simulations. From this figure, the two curves are generally consistent and the peak strengths are also similar. A set of microparameters referred to as the “final sample” is shown for run 2 of Table 5.

### Results and discussion

#### Statistical analysis

The response data were analyzed using Design Expert software to calculate the effects of all of the model terms. Statistical parameters, including the $F$ values, lack of fit, and $R^2$ values, are included in the model. Consequently, a convenient quadratic model is constructed. To calculate the major model terms, insignificant variables and their interactions corresponding to the lowest $F$ values are removed. In this way, the ANOVA results for response 1 (UCS) are summarized in Table 6. For the obtained results, the model accuracy is checked by a lack-of-fit $F$-test. The lack of fit compares the residual error with the pure error. Lack of fit is not desirable, so a small $F$ value and a probability greater than 0.1 are desirable. Models with large lack of fit values are not suitable to predict the investigated response (Ferreira et al., 2007). As shown in Table 6, the lack of fit in the case of the examined model is 1.439, which equates to a probability of greater than 0.1. However, the model is highly significant with a very low probability value (0.0001). The model also shows a very high coefficient of determination $R^2$ (0.962). The $R^2$ value provides a measure of how much variability in the observed response values can be explained by the experimental variables and their interactions. The closer the $R^2$ value is to 1, the better the predicted response obtained by the model (Liu & Chou, 2005). A very low value for the coefficient of variation (e.g., 4.97) indicates the good precision and reliability of the experiments (Zinatizadeh et al., 2006). Adequate precision of 32.123 indicates perfect signal to noise ratio performance and a ratio greater than 4 is acceptable (Körbahti & Rauf, 2008). The predicted sum of squares (PRESS) is a measure of how a particular model fits each point in the design process (Isar, Agarwal, Saran, & Saxena, 2006). Furthermore, Table 6 shows the obtained $p$-value for each variable in the polynomial model of bonded particles. A $p$-value less than 0.05 indicates a good model term, whereas a $p$-value greater than 0.1 indicates a poor model term, which can be ignored.

#### Significant factors

In view of the existing effects between the main factors and the interactions between the two factors, Eq. (7) can be summarized as follows:

$$
Y = b_0 + b_1x_1 + b_2x_2 + b_3x_3 + b_4x_4 + b_5x_5 + b_6x_1^2 + b_7x_2^2 + b_8x_3^2 + b_9x_4^2 + b_{10}x_5^2 + b_{11}x_1x_4 + b_{12}x_2x_3 + b_{13}x_1x_5 + b_{14}x_2x_4 + b_{15}x_3x_5 + b_{16}x_4x_5 + b_{17}x_2x_5 + b_{18}x_4x_5.
$$

Considering the experimental design process in Table 4, experimental results in Table 6, and Eq. (9), the second-order response functions representing the UCS ($Y_1$) and elasticity modulus ($Y_2$) can be expressed as functions of five coded process parameters. As previously mentioned (Table 4), these parameters include the parallel-bond tensile strength (A), parallel-bond cohesion strength (B), parallel-bond effective modulus (C), parallel-bond friction angle [degrees] (D), and parallel-bond stiffness ratio (E). The relationships between the considered responses (the UCS and elasticity modulus) and among the calibration parameters are obtained using the coded and actual variables, presented in Eqs. (11)–(14), respectively.

$$
\text{UCS} = +59.20 + 7.45A - 12.20B - 4.41C + 1.58D + 2.19E + 3.69AB + 1.92AE - 1.49BE + 1.46CD - 2.07A^2 - 2.11B^2 + 2.29C^2 - 1.12E^2,
$$

(11)

$$
\text{UCS} = +1.66065 + 0.21742(pb_ten) + 3.95275(pb_coh) - 2.49864(pb_emod) - 0.18244(pb_FA) + 19.7200(pb_kratio) + 0.14777(pb_ten(pb_coh)) + 0.76875(pb_ten(pb_kratio) - 0.59725(pb_coh(pb_kratio)) + 0.019475(pb_emod(pb_FA) - 0.082704(pb_ten(pb_FA)^2 - 0.084504(pb_coh)^2 + 0.040687(pb_emod)^2 - 4.48042(pb_kratio)^2.
$$

(12)

$$
\text{Elasticity modulus} = +26.48 + 6.91C - 1.67E - 0.47CE - 0.36C^2 + 0.40E^2.
$$

(13)
Table 5
Microparameter levels used for each of the 32 test runs and their results and predicted output values.

<table>
<thead>
<tr>
<th>Run</th>
<th>Independent variable</th>
<th>Predicted output</th>
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<tbody>
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<tr>
<td>14.22</td>
<td>1.93</td>
<td>18.88</td>
</tr>
</tbody>
</table>

Fig. 4. Comparison of the experimental and simulated stress–strain curves.

\[ E = +17.10011 + 1.39194\,(\text{pb_emod}) - 7.53321\,(\text{pb_kratio}) + \\
-0.12433\,(\text{pb_emod})\,(\text{pb_kratio}) - 6.33810 \times 10^{-7}\,(\text{pb_emod})^2 + \\
+1.59393\,(\text{pb_kratio})^2. \]

(14)

In the design process of this experiment, the response factor can be calculated by Eq. (11). The negative signs in front of the variables of the prediction model indicate that to increase the UCS, these factors must be kept at low levels. Fig. 5 shows the studentized residual plots for Y1 (UCS) in the model (Eq. (11)), which includes a comparison of the results for the fitted equation and those obtained from simulation tests. The studentized residual is the residual divided by the estimated standard deviation of that residual. Diagnostic tests are typically performed on studentized residuals to validate the ANOVA. This figure clearly shows that the distribution of the internally studentized residuals for the response approximately follows the fitted normal distribution. Furthermore, from Fig. 5, the inter-
### Table 6
ANOVA results for the response model with the p-value for each variable in the polynomial model.

<table>
<thead>
<tr>
<th>Source</th>
<th>Sum of squares</th>
<th>df</th>
<th>Mean square</th>
<th>F value</th>
<th>p-value (Prob &gt; F)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>6361.887</td>
<td>13</td>
<td>489.3759</td>
<td>61.204</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>$\sigma_t$</td>
<td>1332.805</td>
<td>1</td>
<td>1332.805</td>
<td>166.687</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>$\tau_t$</td>
<td>3571.428</td>
<td>1</td>
<td>3571.428</td>
<td>446.662</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>$\phi$</td>
<td>60.19834</td>
<td>1</td>
<td>60.19834</td>
<td>7.52873</td>
<td>0.0133</td>
</tr>
<tr>
<td>$\mu_{\alpha}/\mu_s$</td>
<td>114.6251</td>
<td>1</td>
<td>114.6251</td>
<td>14.3356</td>
<td>0.0014</td>
</tr>
<tr>
<td>$\mu_{\alpha}/\mu_s$</td>
<td>7.995816</td>
<td>18</td>
<td>7.995816</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\tau_c/\tau_t$</td>
<td>34.13481</td>
<td>1</td>
<td>34.13481</td>
<td>4.269084</td>
<td>0.0535</td>
</tr>
<tr>
<td>$\tau_c/\tau_t$</td>
<td>14.30475</td>
<td>1</td>
<td>14.30475</td>
<td>1.95491</td>
<td>0.1648</td>
</tr>
<tr>
<td>$\tau_c/\tau_t$</td>
<td>154.7195</td>
<td>1</td>
<td>154.7195</td>
<td>19.35006</td>
<td>0.0003</td>
</tr>
<tr>
<td>$\tau_c/\tau_t$</td>
<td>114.6251</td>
<td>1</td>
<td>114.6251</td>
<td>14.3356</td>
<td>0.0014</td>
</tr>
</tbody>
</table>

The adequacy of the established model can also be verified by comparing the results of the PFC based on simulation tests and the constructed equations. It is desirable to obtain a difference of less than 5% (error) between the fitted results and those obtained based on the uniaxial compression simulation. The residuals in Fig. 5 are within this error. Thus, the adequacy of the BPM obtained based on microparameter analysis for representing the mechanical properties of rock material is confirmed. Fig. 6(a)–(d) shows the 3D response surface plots obtained from the simulation results using Eq. (11), which describe the effect of the process variables on the UCS behavior.
Discussion of the influence of the microparameters on the macrobehavior

Zhang (2010) proposed a simple sensitivity analysis to understand the cross-influence of microparameters regarding the global mechanistic behavior of the specimen. In the established framework, a set of microparameters referred to as the “final sample” are derived based on trial and error to reproduce the results from reference lab tests. Based on the final sample, a parametric analysis is then performed. This technique is implemented here by changing...
one microparameter at the time and inspecting the strain–stress response. The influences of all of the independent microparameters (changed one at a time) are summarized in Fig. 7. The developed approach for parametrical analysis generally requires numerous model runs and hence takes a long time to obtain an appropriate set of results. Here, DOE is applied to sensitivity analysis of the microparameters of the BPMs.

**Effect of the parallel-bond effective modulus**

The parallel-bond normal effective modulus \( \overline{E} \) is the normal Young’s modulus at each parallel-bond contact. As shown in Fig. 6(c), the peak strength of the sample tends to slightly decrease with increasing parallel normal \( \overline{E} \). However, the parallel bond would break at a smaller strain for higher bond \( \overline{E} \). Consequently, the peak strength exhibits decreasing behavior and the post peak behavior encounters a lower stress level. Fig. 8 shows the effect of the parallel-bond effective modulus on the elasticity modulus. From this figure, it is suggested that this microparameter also changes the initial elastic response of the sample. Increasing this microparameter moves the initial elastic linear line upwards, and hence makes the sample more difficult to deform.

**Effect of the parallel-bond normal to shear stiffness ratio**

The parallel-bond normal to shear stiffness ratio \( (k_n/k_s) \) is defined as the ratio of the normal Young’s modulus to the shear bond Young’s modulus. This ratio indirectly reflects the level of the parallel-bond shear stiffness. Fig. 9(a) shows that increasing this ratio would decrease the initial elasticity. Specifically, it indicates an inverse relationship between this microparameter and the material elasticity modulus. As shown in Fig. 6(b) and (d), Fig. 9(b) shows that increasing this ratio (i.e., increasing the parallel-bond tensile strength and parallel-bond cohesion strength) increases the UCS.

**Effect of the parallel-bond tensile strength**

The parallel-bond tensile strength is defined as the normal strength of the cement-like material, which is characterized by the parallel-bond model. It is shown that the value of the parallel tensile strength slightly affects the initial linear elastic behavior of the sample. In contrast, its influence on the peak strength of the sample is remarkable, as shown in Fig. 10(a).

**Effect of the parallel-bond cohesion strength**

As shown in Fig. 5, increasing the parallel-bond cohesion strength increases the peak strength (i.e., the UCS). When the par-
Parallel shear strength is relatively large, the parallel normal tensile strength effectively increases the peak strength. The relationship between the parallel tensile strength and the cohesion strength suggests the failure mechanism in the parallel-bond model by controlling the crack types.

Effect of the particle to particle friction angle

Fig. 10(b) shows that the particle friction angle does not greatly influence the behavior of the sample. There is only a slight change in the post peak behavior with a change in the particle friction angle.

Conclusions

In this study, we used the response surface methodology (RSM) and central composite design (CCD) to analyze the possible influence and interactions between microparameters in a bonded particle model (BPM) calibration process. The investigated parameters included the parallel-bond tensile strength, parallel-bond cohesion strength, parallel-bond effective modulus, parallel-bond friction angle, and parallel-bond stiffness ratio. Numerical simulations were performed and the obtained results were carefully analyzed. Using a set of experimental data and a mathematical software package (Design Expert), a mathematical model equation was derived for the UCS and elasticity modulus. To incorporate the effect of microparameters on the macroparameter behavior, 3D response surface plots were constructed. The predicted values based on the proposed model were in good agreement with the observed values ($R^2 = 0.962$ for the UCS). Some of the notable observations for the proposed approach are as follows:

- The parallel-bond stiffness has a direct influence on the peak strength behavior of the sample. This also reveals an inherent effect on breakage of parallel bonds.
- The existent friction coefficient in the contact bond has little influence on the behavior of the sample.
- Considering the influence of the remaining parameters, simple mechanical indicators, such as the elasticity modulus and peak strength, are not affected by a single parameter. Specifically, the elasticity modulus is related to both the particle normal shear stiffness and the parallel-bond normal shear stiffness. Furthermore, fluctuation of the peak strength seems to be related to all five parameters.
- The two most significant microparameters that affect the UCS are the parallel-bond tensile strength and parallel-bond cohesion strength. This can be intuitively understood as the stronger the bond strength, the better the model can resist bond breaking and propagation.

- The elasticity modulus is highly correlated with the particle-scale contact modulus.

References


