

Article

Analysis of the Mechanism of Main Effects of Microscopic Parameters on Macroscopic Parameters in the PFC^{2D} Parallel Bonding Model

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Abstract

To establish a quantitative mapping relationship between macro- and micro-parameters in the PFC^{2D} parallel bonding model, and in view of the inherent complexity of the mutual validation process between laboratory experiments and parameter calibration, this paper takes uniaxial compression tests as the mechanical reference. By combining orthogonal experimental design, Pearson correlation analysis and multivariate analysis of variance, this study systematically investigates the effects of 10 micro-parameters on 6 macro-mechanical indicators (modulus of elasticity E , Poisson's ratio ν , uniaxial compressive strength σ_c , friction-to-cohesion ratio FCR , crack initiation strength σ_{ci} and crack damage stress σ_{cd}). To reduce the coupling dimension between cohesion and internal friction angle in the calibration of PFC macro-micro parameters, this paper defines the Friction-to-Cohesion Ratio (FCR) as the ratio of the equivalent macroscopic angle of internal friction to the equivalent macroscopic cohesion, and systematically conducts sensitivity analyses of uniaxial compression simulations. The results indicate that the elastic modulus E is primarily governed by E^* , $\bar{E}^*$, $\bar{k}^*$ and R_f ; the Poisson's ratio ν is mainly influenced by E^* , k^* , $\bar{E}^*$, $\bar{k}^*$ and R_f ; the uniaxial compressive strength σ_c , the crack initiation strength σ_{ci} and the crack damage stress σ_{cd} are primarily regulated by $\bar{\sigma}_c$ and R_f ; whilst the Friction-to-Cohesion Ratio (FCR) is mainly affected by $\bar{\sigma}_c$, $\bar{\varphi}$, R_f , $\bar{c}$ and β ; Elasticity parameters and strength parameters are governed by different micro-mechanisms, reflecting the fundamental decoupling of stiffness and strength in the PFC model. This study established a progressive 'screening-validation-quantification' sensitivity analysis framework, revealing the directional regulation patterns of various micro-parameters on macroscopic responses, thereby providing a theoretical basis for the targeted optimisation and efficient calibration of micro-parameters in PFC discrete element simulations.

Keywords: parallel bonding model; macro-micro parameter mapping; orthogonal experimental design; Pearson correlation analysis; multi-factor analysis of variance



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1. Introduction

In the discrete element method (DEM)-based particle flow code PFC^{2D}, parameter calibration is a crucial step in bridging the numerical model with physical reality. When conducting numerical simulations using a discrete element model, each particle-particle contact model involves multiple microscopic parameters. When selecting a particle-particle contact model, it is often necessary to define a large number of micro-parameters. To

ensure that the macroscopic mechanical properties exhibited by the particle aggregate closely resemble those of the simulated soil and rock materials, it is crucial to investigate the relationship between micro- and macro-parameters and to utilise these relationships to calibrate the macro- and micro-parameters [1].

Many scholars in China have conducted research on the influence of macro–micro parameters and parameter calibration in discrete element method (DEM) software. Huang et al. [2] analysed the entire micro-evolutionary mechanism of strength deviation in rock samples simulated by the PBM method, which can provide a reference basis for future research to analyse and interpret a large volume of early PBM simulation results; Zhou et al. [3] employed two multivariate non-linear fitting equations to quantitatively describe the combined relationship between various micro-parameters and the material's macroscopic shear strength parameters, and provided recommended values for the K-value (tangential bond strength/normal bond strength); Abir et al. [4] employed the control variable method to conduct a relatively comprehensive analysis of the quantitative relationships between micro-parameters and macro-parameters; taking into account the mutual influence of parameters, they fitted empirical equations and optimised the selection of micro-parameters. Miao et al. [5] conducted a qualitative study based on the Plackett–Burman (PB) design to analyse the stress conditions in the vertical diameter of a Brazilian disc. They established a theoretical relationship between rock tensile strength and microstructural strength parameters. Using the results of numerical simulations, they modified the aforementioned theoretical equations and derived modified equations for rock tensile strength and microstructural strength parameters; Liu et al. [6] investigated the mechanical strength and failure characteristics of coal samples through uniaxial compression tests under different quasi-static loading rates (ranging from 0.0005 mm/s to 0.01 mm/s), combining high-speed digital image correlation (DIC) technology with numerical simulation; Zou and Lin et al. [7] proposed a GT-RSM -MD combined optimisation method; through grey correlation analysis and factor screening, they established a response surface model relating three macroscopic parameters to their governing microscopic parameters; Ren et al. [8] proposed an improved BP algorithm to quantify the sensitivity between macroscopic and microscopic parameters, obtained a non-linear model of macro-microscopic parameters described by multiple sub-response surfaces, established a mathematical model for parameter calibration, and obtained the optimal solution for rock intermediate layer parameters through optimisation techniques; Wu and Huang et al. [9] investigated the strength and failure modes of rock with non-linear cracks. Based on calibrated PBM and FJM parameters, they constructed a PFC model, further discussing the crack inclination, stress distribution within the specimen, and the evolution of local stresses around the crack, whilst summarising the advantages and disadvantages of the two contact models. Xue and Li et al. [10] investigated the internal damage of granite induced by liquid nitrogen (LN2) cold shock using X-ray computed tomography (CT) technology. Traditional threshold segmentation methods are subjective and may obscure subtle grayscale variations. In contrast, the Gray Level Co-occurrence Matrix (GLCM), based on second-order statistical measures of grayscale values, quantifies texture features and captures comprehensive fracture information. Uniaxial compression tests were performed on granite samples subjected to cyclic heating and LN2 treatment, followed by X-ray CT scanning. Image processing techniques and GLCM were employed to extract key features from CT images. Statistical analysis was conducted to quantify the cracks and micro-damages in granite induced by LN2 cold shock; Li and Zhu et al. [11] investigate the evolution of macro-mechanical properties and fracture structures in granite subjected to repeated high-temperature heating and LN2 cryogenic impact cycle conditions simulating artificial thermal reservoir stimulation in

hot dry rock environments. Standardized granite specimens were treated with varying thermal–cryogenic cycles followed by comprehensive characterization at multiple scales.

In summary, the specific methods for calibrating the micro-parameters and macroscopic mechanical parameters of rock mass materials warrant further investigation. To better utilise given macroscopic rock mass parameters to match corresponding micro-parameters, this paper employs the PFC^{2D} discrete element software, based on uniaxial compression tests and existing strength theories in rock mechanics. Addressing the issue of strong coupling between cohesion and internal friction angle in the calibration of PFC macro- and micro-parameters, this study innovatively proposes the Friction-to-Cohesion Ratio (*FCR*) as a comprehensive indicator, reducing the two-dimensional parameter space to one dimension. Subsequently, by designing orthogonal experiments to analyse the sensitivity of principal effects, an optimised macro-micro parameter calibration workflow was obtained.

2. Establishment of the Parallel Bonding Model and Specimen Model

The PFC software provides ten built-in particle contact models, including the empty model, linear model, linear contact-bonding model, linear parallel bonding model, Hertzian contact model, hysteretic damping model, smooth joint model, flat joint model, anti-rolling linear contact model, and Burgers creep model. Among these, the linear model, linear contact-bonded model and linear parallel-bonded model are the most commonly used contact models. The linear parallel-bonded model comprises two types of parallel contact interfaces: one is a linearly elastic interface that cannot withstand tensile or torsional forces, but can only withstand compressive and frictional forces; the other is a linearly elastic bonded interface capable of transmitting forces and moments, as shown in Figure 1a. The linear contact-bonding model can only exist in one of two states: bonded or unbonded. When bonded, the interface cannot withstand frictional forces; once the bonding link breaks, the interface transitions to an unbonded state, at which point it can support sliding provided the shear force satisfies the Coulomb criterion, as shown in Figure 1b. Both the linear parallel bonding model and the linear contact bonding model degrade to a linear model after the bond breaks [12].

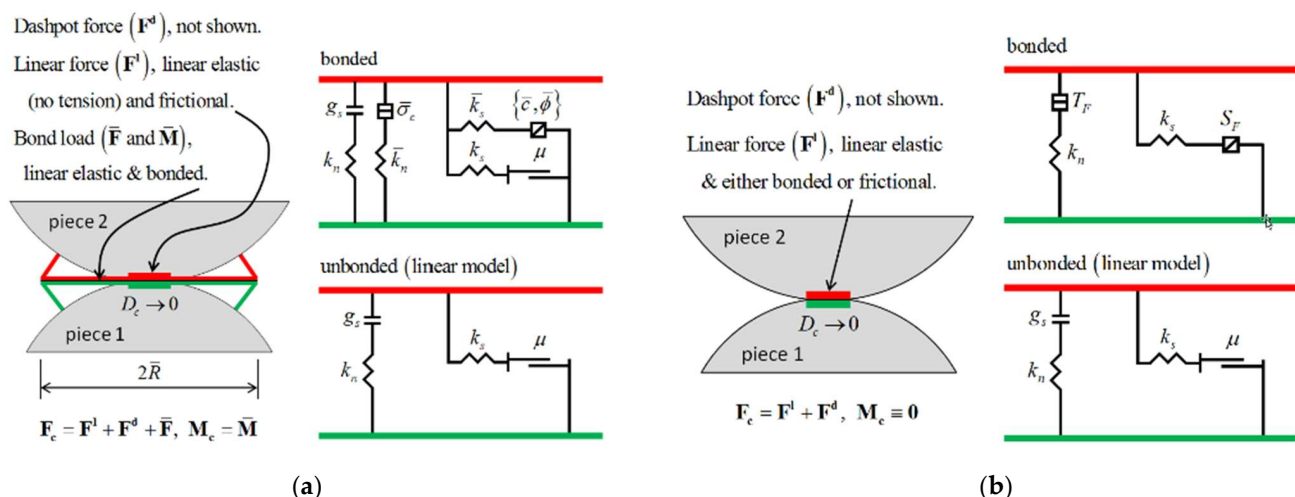


Figure 1. Particle contact model: (a) Linear parallel bonding model; (b) Linear contact bonding model.

As the linear parallel bonding model is capable of simultaneously transmitting both force and moment, it better reflects the forces within an intact rock mass and is suitable for simulating materials with high bond strength, such as reinforcing bars, rock and concrete; whereas the linear model or linear contact bonding model is more suitable for simulating

soil. Therefore, the linear parallel bonding model is adopted in this study to simulate the entire process of rock failure.

In accordance with the suggested methods of the International Society for Rock Mechanics [13], the model dimensions were set at 50 mm × 100 mm, with the minimum particle size taken as 1/100 of the model diameter and the particle size ratio set at 1.66. The PFC model is shown in Figure 2.

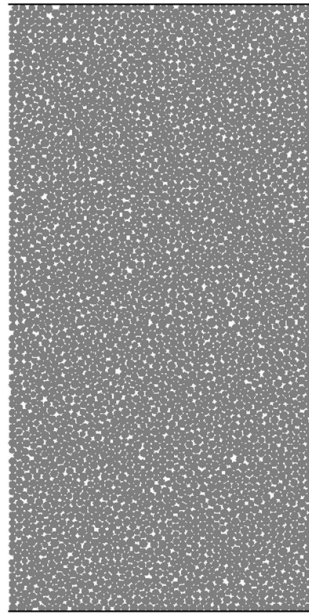


Figure 2. PFC model of the specimen.

3. Orthogonal Experimental Design

3.1. Principles of Orthogonal Experimental Design

In scientific experiments, it is common for test results to be influenced by multiple factors. If a comprehensive testing approach were adopted, the workload would increase exponentially with the number of factors. Orthogonal experimental design is an optimised experimental method that utilises orthogonal tables to scientifically arrange factor combinations, enabling the attainment of highly reliable experimental results whilst significantly reducing the number of trials. Through multi-factor analysis of variance, the degree of influence of numerous factors on experimental indicators can be assessed. Therefore, the orthogonal experimental design method was adopted to investigate the relationship between macroscopic and microscopic parameters in the PFC^{2D} parallel bonding model, quantifying the corresponding relationships between parameters to provide a basis for parameter calibration [14].

In orthogonal experimental design, the subject and scope of the experimental study are jointly determined by factors and levels. Here, factors refer to independent variables that may influence the experimental results; levels refer to the different states or values that a particular factor assumes in the experiment.

An orthogonal array is a fundamental tool for arranging experiments and analysing results in orthogonal experimental design, generally denoted as $L_n(m^k)$. Here, L is the orthogonal array code; n is the number of trials; m is the number of levels for each factor; and k is the number of factors [15].

Orthogonal tables possess two important properties: uniformity of distribution and uniformity of comparison. Uniformity of distribution refers to the fact that the experimental schemes selected by the orthogonal table are uniformly distributed across the entire exper-

imental space, with the combinations of levels in any two columns being complete and occurring with equal frequency; uniformity of comparison refers to the fact that the structure of the orthogonal table is regular, symmetrical and orderly, with each level in every column occurring exactly the same number of times, thereby ensuring good comparability between different levels.

3.2. Pearson Correlation Analysis

Pearson correlation analysis is a statistical method used to measure the strength and direction of the linear relationship between two continuous variables. Its fundamental principle is based on the ratio of covariance to the standard deviation of the variables. It quantifies the degree of co-variation between two variables by calculating the correlation coefficient r , which ranges from -1 to $+1$. The closer the absolute value is to 1, the stronger the linear relationship; a positive value indicates a positive trend, whilst a negative value indicates an inverse trend. The basic assumptions of this method include that both variables are continuous and follow an approximate normal distribution; that the relationship between the variables is linear rather than curvilinear; that the data consist of independent, paired observations; and that there are no significant outliers. Pearson correlation is suitable for analysing scenarios such as linear associations between continuous variables, provided the data satisfy the above assumptions [16]. The formula is

$$r = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^n (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^n (Y_i - \bar{Y})^2}} \quad (1)$$

where the numerator is the sum of the products of the deviations from the mean for both variables (i.e., the covariance), and the denominator is the geometric mean of the sums of the squares of the deviations from the mean for both variables. Standardisation is applied to eliminate the influence of units, ensuring that the result reflects only the relative strength of the linear relationship [17]. Pearson correlation analysis can be used to preliminarily identify significant influencing factors prior to conducting a multi-factor analysis of variance.

3.3. Multifactorial Analysis of Variance

Multifactor analysis of variance is a statistical method that, building upon single-factor analysis, simultaneously examines the effects of two or more categorical independent variables on the mean of a continuous dependent variable, whilst revealing interactions between factors. Its fundamental principle involves decomposing the total variance of the dependent variable into three components according to different sources: the main effects of each factor, the interaction effects between factors, and random error. By comparing the mean squares of different sources with the mean square error, an F-statistic is constructed to test whether the main effects and interaction effects are significantly non-zero; This method requires that the dependent variable follow a normal distribution within each group with homogeneity of variance, that the observations are independent of one another, that the factors are categorical variables whilst the dependent variable is continuous, and that the sample size in each cell meets certain requirements to ensure statistical power; multifactorial analysis of variance is suitable for experimental designs where multiple categorical independent variables are manipulated simultaneously to observe their effects on a continuous dependent variable [18]. It enables the distinction, within a single analysis, between the independent contributions of each factor and their synergistic or antagonistic effects, thereby enhancing research efficiency and better reflecting the complex reality of multiple variables acting in concert.

4. Experimental Parameters and Factors

4.1. Selection of Test Parameters

Rock mechanics testing assesses the failure modes and deformation characteristics of rock under various loading conditions. Through such testing, mechanical parameters of rock materials can be obtained, including compressive strength, elastic modulus, Poisson's ratio and cracking strength. To cover fundamental mechanical properties, compressive strength, elastic modulus and Poisson's ratio were selected as test parameters.

Currently, most studies on parameter calibration are based on uniaxial compression tests [9,19–21], involving the continuous adjustment of micro-parameters to fit stress–strain curves. However, such methods can only yield elastic and strength parameters such as elastic modulus, Poisson's ratio and uniaxial compressive strength; they cannot directly determine cohesion and angle of internal friction, which reflect the material's shear failure characteristics. Abir et al. [4] noted that, as the vast majority of rocks in nature are subjected to triaxial stress conditions, traditional approaches require separate triaxial compression simulations to calibrate these parameters; however, this significantly increases computational costs and the complexity of parameter optimisation. To extract shear strength parameters within a uniaxial compression framework, this paper utilises PFC uniaxial simulation results. By tracking the morphology of the specimen's macroscopic fracture surface following peak stress, the failure angle β (i.e., the angle between the fracture surface and the direction of the maximum principal stress) is precisely measured during the PFC simulation. Subsequently, based on the intrinsic relationship between the failure angle and the angle of internal friction in Mohr–Coulomb theory

$$\varphi = 90^\circ - 2\beta \quad (2)$$

to calculate the equivalent angle of internal friction obtained during the simulation. This value is then substituted into the formula for uniaxial compressive strength

$$\sigma_c = \frac{2c \times \cos \varphi}{1 - \sin \varphi} \quad (3)$$

to solve for the equivalent cohesion, thereby establishing a theoretical link between the uniaxial simulation and the shear strength parameters. It should be noted that this method implicitly assumes that the rock obeys the Mohr–Coulomb failure criterion and that the failure plane is planar. Its uncertainties primarily stem from the subjectivity of failure angle measurements (such as fluctuations in inclination caused by local undulations in the fracture surface), the dynamic nature of fracture surface evolution during the post-peak stress decay process, and the discrepancy in boundary conditions arising from the fact that, whilst lateral stress is zero under uniaxial conditions, actual rock masses are predominantly subjected to triaxial stress states; To address this, this study statistically averaged the failure angles of multiple specimens under the same operating conditions to reduce variability, and explicitly defined the obtained parameters as equivalents of macroscopic parameters—that is, calibrated parameters characterising the macroscopic shear strength properties of the aggregate, rather than the physical constants of the actual rock. Nevertheless, cohesion and the angle of internal friction, as two independent strength parameters, exhibit significant non-linear coupling characteristics during the adjustment of PFC micro-parameters—different (c, φ) combinations may yield similar uniaxial compressive strengths, leading to a dilemma of high-dimensional coupling and multiple solutions in parameter sensitivity analysis.

To overcome this bottleneck, this paper proposes the Friction-to-Cohesion Ratio (*FCR*) as a comprehensive indicator, defined as the ratio of the equivalent angle of internal friction to the equivalent cohesion, i.e.,

$$FCR = \frac{\varphi^*}{c^*} \quad (4)$$

where,

FCR is the friction-to-cohesion ratio, °/MPa;

φ^* is the equivalent internal friction angle, °;

c^* is the equivalent cohesion, MPa.

By reducing the two-dimensional strength parameter space to one dimension, this parameter effectively decouples the synergistic effects of cohesion and the angle of internal friction. Its physical significance lies in characterising the degree to which a material's internal friction properties dominate over its cohesion properties—a low *FCR* value indicates that strength is primarily contributed by cohesion and that failure is predominantly brittle tensile, whereas a high *FCR* value implies that friction mechanisms predominate and shear slip characteristics are pronounced. In terms of theoretical consistency, the *FCR* is derived from the uniaxial strength expression based on the Mohr–Coulomb criterion. Under the constraint of uniaxial compressive strength, it has a one-to-one correspondence with the (*c*, φ) combination, ensuring the uniqueness of parameter inversion; In terms of methodological necessity, the introduction of *FCR* transforms the sensitivity analysis of macro- and micro-parameters from the traditional approach of ‘examining the influence of *c* and φ on the macroscopic response separately’ to ‘systematically revealing the intrinsic laws governing the mechanisms by which micro-parameters regulate material strength composition’. This significantly enhances the efficiency and physical interpretability of parameter determination; therefore, the cohesion ratio *FCR* is employed as the experimental indicator in this paper.

Crack initiation strength serves as an indicator of crack initiation and stable propagation [22]; it is of significant importance for estimating the extent of the loosened zone in rock tunnels and guiding rock mass support. In laboratory testing, the crack initiation strength of rock specimens is typically determined by calculating the volumetric strain of the crack or by combining results from acoustic emission tests. The use of PFC to simulate rock specimens allows the number of cracks and their propagation during the loading process to be recorded, enabling the crack initiation strength to be determined based on the number of cracks. Therefore, crack initiation strength is selected as a test parameter.

During uniaxial compression, rock failure does not occur instantaneously but proceeds through multiple stages, including the elastic stage, stable crack propagation, unstable crack propagation, and post-peak failure. Furthermore, the crack damage stress typically corresponds to the critical point at which crack propagation transitions from stable to unstable, marking the onset of significant accumulation of macroscopic damage in the rock. Compared to peak strength, crack damage stress better reflects the changes in the mechanical response of rock prior to failure [23], such as the onset of a decrease in elastic modulus, an increase in Poisson's ratio, and a rapid increase in the number of microcracks. These changes serve as a bridge between macroscopic mechanical parameters (such as elastic modulus and Poisson's ratio) and microscopic parameters (such as bond strength and friction coefficient), and are therefore of significant reference value in parameter calibration. Consequently, crack damage stress is selected as the test parameter.

In summary, this paper selects elastic modulus, Poisson's ratio, uniaxial compressive strength, friction-to-cohesion ratio, crack initiation stress and crack damage stress as the test indicators for the correlation analysis of parameters.

4.2. Determination of Experimental Factors

The Parallel Bonding Model (PBM) is employed to simulate rock laboratory tests. The Parallel Bonding Model represents rock as an assembly of discs of finite thickness, connected by bonding links; the contacts between discs and the bonding regions possess finite stiffness. When the applied local stress (i.e., tensile stress, shear stress or torsional moment) exceeds the specified strength of the links, these links rupture, forming a microcrack. In this process, the PFC does not require any description of post-yield flow behaviour to control fracture behaviour; it only requires the motion laws of the particles, simple constitutive laws for particle deformation, and yield laws for particle bond failure. The parameters of the Parallel Bonded Model primarily include particle-scale parameters and bond-scale parameters, as detailed in Table 1.

Table 1. Main macro- and mesoscale mechanical parameters of the PFC^{2D} model.

Category	Parameter	Symbol
Particle Microscopic Parameters	Relative particle radius	$L/R_{\min}$
	Particle size ratio	$R_{\max}/R_{\min}$
	Particle density/($kg \cdot m^3$)	ρ
	Effective elastic modulus of the particle/GPa	E^*
	Particle method tangential stiffness ratio	k^*
	Particle surface friction coefficient	μ
Binding microstructural parameters	Effective elastic modulus of parallel bonding/GPa	$\bar{E}^*$
	Parallel bonding method tangential stiffness ratio	$\bar{k}^*$
	Parallel bonding tensile strength/MPa	$\bar{\sigma}_c$
	Shear strength of parallel bonding/MPa	$\bar{c}$
	Parallel bond friction angle/(°)	$\bar{\varphi}$
	Moment distribution coefficient	β
	Filler ratio	R_f
	Normal bond stiffness/MPa	k_n^b
Macroscopic parameters	Shear bond stiffness/MPa	k_n^s
	Uniaxial compressive strength/MPa	σ_c
	Modulus of elasticity/GPa	E
	Poisson's ratio	ν
	Internal friction angle/(°)	φ
	Cohesion/MPa	c
	Crack initiation strength/MPa	σ_{ci}
	Crack damage intensity/MPa	σ_{cd}
	friction-to-cohesion ratio/(°/MPa)	FCR

Following the recommendations of POTYONDY et al. [24] regarding the calibration of mesoscale parameters, certain assumptions were made regarding these parameters. Zhao et al. [25] conducted research on the particle size ratio (i.e., the ratio of the largest particle radius to the smallest particle radius in the model, $R_{\max}/R_{\min}$) and concluded that when the particle size ratio is set between 1 and 5, it has virtually no effect on the mechanical properties of the model. Consequently, following the recommended value proposed by POTYONDY et al., the particle size ratio was set to a constant value of 1.66. As this paper aims to investigate in detail the differences in the calibration of mesoscale parameters within the parallel bonding model, it no longer assumes that particles and bonding bonds share a common microscopic elastic modulus; however, regarding the choice of stiffness

ratio, it still adopts the recommendation of POTYONDY et al. regarding the calibration of microscopic parameters, namely $E^* \neq \bar{E}^*$, $k^* \neq \bar{k}^*$. Based on the above assumptions and the fundamental principles of the PFC model, the microscopic parameters of the particle flow were simplified and adjusted, and ultimately the following 10 microscopic parameters were selected as experimental factors: E^* , k^* , $\bar{E}^*$, $\bar{k}^*$, $\bar{\sigma}_c$, $\bar{c}$, $\bar{\varphi}$, μ , β , R_f .

4.3. Range of Test Parameters

Research by Deng Shuxin et al. [26] indicates that the Poisson's ratio of rock materials is related to the stiffness ratio. By setting all parameters other than the stiffness ratio to constant value $E^* = 8.0$ GPa, $\bar{E}^* = 8.0$ GPa, $\bar{\sigma}_c = 25.5$ MPa, $\bar{c} = 78.1$ MPa, $\bar{\varphi} = 30.0^\circ$, $\mu = 0.577$, $\beta = 0.3$, $R_f = 1.0$, $\rho = 2500$ kg·m³, and setting k^* and $\bar{k}^*$ to 0.2–0.8, a series of uniaxial compression tests were conducted; fitting the test results yields the relationship between the stiffness ratio and the Poisson's ratio;

$$\nu = -0.067 + 0.231k^* - 0.035k^{*2} \quad (5)$$

Existing data provide a statistical summary of the Poisson's ratios for common rocks, indicating that most values fall between 0.1 and 0.4. Substituting $\nu = 0.1$ and $\nu = 0.4$ into the formula for the relationship between the stiffness ratio and the Poisson's ratio given above yields $k^* = 0.82$ and $k^* = 5.80$, respectively; therefore, the range of stiffness ratios is set to 2.0–6.0.

Other mesoscale parameters were also determined through similar calculations: the effective elastic modulus of the particles (E^*) was set within the range of 1.0–5.0 GPa; the effective elastic modulus of parallel bonding ($\bar{E}^*$) was set within the range of 1.5–4.5 GPa; and the torque distribution coefficient (β) was set within the range of 1.2–1.6.

In the discrete element model (DEM), the slip between particles following bond failure is related to the friction coefficient μ . POTYONDY et al. suggest that the friction coefficient may influence the post-peak behaviour of the material and recommend setting μ to 0.5 for rock materials. To investigate the influence of μ on macroscopic parameters, the range of μ was set to 0.5–0.9, which is similar to the values reported in the literature [24,25,27].

The parallel bond tensile strength and parallel bond shear strength are closely related to the failure mode of the model. When the parallel bond tensile strength is too high, the model exhibits the mechanical properties of a ductile material, with failure at the microscopic level dominated by shear cracks; when the parallel bond shear strength is too high, the model exhibits more of the characteristics of a brittle material at the macroscopic level, and transverse tensile failure caused by the Poisson effect often occurs [27]. Based on this theory, the range of values for the parallel bond tensile strength $\bar{\sigma}_c$ was set at 4.5–9.5 MPa, and the range of values for the parallel bond shear strength $\bar{c}$ was set at 10–20 MPa.

Chen et al. [28] conducted research on the relationship between the parallel bonding friction angle $\bar{\varphi}$ and macroscopic mechanical parameters using uniaxial or triaxial numerical tests. Based on their findings, the value of $\bar{\varphi}$ was set to 10–50°.

The filler ratio, as a micro-scale parameter, represents the ratio of the actual radius of the bonding surface to the geometric contact radius between two particles [19]. Consultation of the manual indicates that this parameter should not be set below 0.60; otherwise, the bonding surface becomes too small, leading to a sharp drop in the elastic modulus and excessive brittleness in the post-peak curve. Based on this, the range for the filler ratio R_f is set to 0.8–1.2.

5. Sensitivity Analysis of Microscopic Parameters

5.1. Orthogonal Experimental Design Scheme and Computational Results

Based on the previous discussion regarding the selection of experimental factors and indicators, the following 10 micro-parameters have been selected as experimental factors: E^* , k^* , $\bar{E}^*$, $\bar{k}^*$, $\bar{\sigma}_c$, $\bar{c}$, $\bar{\varphi}$, μ , β , and R_f . The following seven macro-parameters have been selected as experimental indicators: σ_c , E , ν , FCR, σ_{ci} , and σ_{cd} . For each experimental factor, three appropriate levels have been selected based on their range of values. Based on the number of factors and their levels, an orthogonal table design ($L_{27}(3^{13})$) was adopted for the experiment. According to the factor levels, 27 parameter combinations can be set up, with the last three columns serving as dummy columns. The range (or variance) corresponding to these dummy columns can be treated as pure experimental error (Se), which is used to calculate the F-value, ensuring that random fluctuations in the data are not mistaken for treatment effects when assessing the significance of other factors.

The table of factor levels is shown in Table 2. The orthogonal numerical experimental design is shown in Table 3.

Table 2. Table of factor levels.

No.	E^* (GPa)	k^*	$\bar{E}^*$ (GPa)	$\bar{k}^*$	$\bar{\sigma}_c$ (MPa)	$\bar{c}$ (MPa)	$\bar{\varphi}$ (°)	μ	β	R_f
1	1.0	2.0	1.5	2.0	4.5	10.0	10.0	0.5	1.2	0.8
2	3.0	4.0	3.0	4.0	7.0	15.0	30.0	0.7	1.4	1.0
3	5.0	6.0	4.5	6.0	9.5	20.0	50.0	0.9	1.6	1.2

Table 3. Orthogonal numerical test plan.

No.	E^* (GPa)	k^*	$\bar{E}^*$ (GPa)	$\bar{k}^*$	$\bar{\sigma}_c$ (MPa)	$\bar{c}$ (MPa)	$\bar{\varphi}$ (°)	μ	β	R_f	Factor 11	Factor 12	Factor 13
1	1.0	2.0	1.5	2.0	4.5	10.0	10.0	0.5	1.2	0.8	(empty column)		
2	1.0	2.0	1.5	2.0	7.0	15.0	30.0	0.7	1.4	1.0			
3	1.0	2.0	1.5	2.0	9.5	20.0	50.0	0.9	1.6	1.2			
4	1.0	4.0	3.0	4.0	4.5	10.0	10.0	0.7	1.4	1.0			
5	1.0	4.0	3.0	4.0	7.0	15.0	30.0	0.9	1.6	1.2			
6	1.0	4.0	3.0	4.0	9.5	20.0	50.0	0.5	1.2	0.8			
7	1.0	6.0	4.5	6.0	4.5	10.0	10.0	0.9	1.6	1.2			
8	1.0	6.0	4.5	6.0	7.0	15.0	30.0	0.5	1.2	0.8			
9	1.0	6.0	4.5	6.0	9.5	20.0	50.0	0.7	1.4	1.0			
10	3.0	2.0	3.0	6.0	4.5	15.0	50.0	0.5	1.4	1.2			
11	3.0	2.0	3.0	6.0	7.0	20.0	10.0	0.7	1.6	0.8			
12	3.0	2.0	3.0	6.0	9.5	10.0	30.0	0.9	1.2	1.0			
13	3.0	4.0	4.5	2.0	4.5	15.0	50.0	0.7	1.6	0.8			
14	3.0	4.0	4.5	2.0	7.0	20.0	10.0	0.9	1.2	1.0			
15	3.0	4.0	4.5	2.0	9.5	10.0	30.0	0.5	1.4	1.2			
16	3.0	6.0	1.5	4.0	4.5	15.0	50.0	0.9	1.2	1.0			
17	3.0	6.0	1.5	4.0	7.0	20.0	10.0	0.5	1.4	1.2			
18	3.0	6.0	1.5	4.0	9.5	10.0	30.0	0.7	1.6	0.8			
19	5.0	2.0	4.5	4.0	4.5	20.0	30.0	0.5	1.6	1.0			

Table 3. Cont.

No.	E^* (GPa)	k^*	$\bar{E}^*$ (GPa)	$\bar{k}^*$	$\bar{\sigma}_c$ (MPa)	$\bar{c}$ (MPa)	$\bar{\varphi}$ (°)	μ	β	R_f	Factor 11	Factor 12	Factor 13
20	5.0	2.0	4.5	4.0	7.0	10.0	50.0	0.7	1.2	1.2			
21	5.0	2.0	4.5	4.0	9.5	15.0	10.0	0.9	1.4	0.8			
22	5.0	4.0	1.5	6.0	4.5	20.0	30.0	0.7	1.2	1.2			
23	5.0	4.0	1.5	6.0	7.0	10.0	50.0	0.9	1.4	0.8			
24	5.0	4.0	1.5	6.0	9.5	15.0	10.0	0.5	1.6	1.0			
25	5.0	6.0	3.0	2.0	4.5	20.0	30.0	0.9	1.4	0.8			
26	5.0	6.0	3.0	2.0	7.0	10.0	50.0	0.5	1.6	1.0			
27	5.0	6.0	3.0	2.0	9.5	15.0	10.0	0.7	1.2	1.2			

Tests were conducted sequentially based on the above combinations of parameters; the test specimens are shown in Figure 2. The data obtained from the tests for each set of parameters have been compiled into the orthogonal experimental results shown in Table 4.

Table 4. Orthogonal experimental results.

No.	E/GPa	ν	σ_c/MPa	$FCR/(\text{°}/\text{MPa})$	σ_{ci}/MPa	σ_{cd}/MPa
1	1.77	0.24	7.19	12.68	3.21	6.92
2	2.15	0.22	13.30	10.94	6.28	12.82
3	2.46	0.20	20.11	6.49	13.41	19.09
4	2.96	0.31	7.74	10.50	3.97	7.48
5	3.45	0.29	13.86	7.66	7.39	13.53
6	2.50	0.33	12.82	5.15	6.69	12.75
7	4.37	0.33	7.99	10.18	4.52	7.94
8	3.15	0.36	8.91	15.40	4.96	8.74
9	3.78	0.35	14.39	5.01	8.25	14.20
10	4.43	0.38	9.19	25.97	5.02	9.10
11	3.73	0.39	8.25	15.66	4.03	8.12
12	4.70	0.34	23.71	4.67	12.71	23.53
13	5.11	0.26	6.23	39.40	2.66	6.14
14	6.08	0.24	15.27	4.11	6.89	15.19
15	6.83	0.22	21.25	9.48	10.89	20.77
16	2.99	0.47	8.77	25.01	4.57	8.74
17	3.18	0.45	14.58	6.04	9.14	14.51
18	2.68	0.51	11.55	11.53	5.40	11.38
19	6.51	0.35	7.39	16.79	3.68	7.21
20	7.44	0.31	16.61	10.53	9.37	16.60
21	6.09	0.33	12.92	4.01	5.99	12.83
22	4.13	0.51	10.62	16.62	5.92	10.54
23	3.65	0.59	9.06	10.00	4.43	9.06
24	3.77	0.58	13.76	8.48	7.96	13.58
25	4.62	0.38	7.06	27.23	3.24	6.87
26	5.78	0.35	12.08	13.80	5.65	11.95
27	6.43	0.32	24.70	2.34	13.08	24.38

5.2. Analysis of the Results of an Orthogonal Experiment

5.2.1. Calculation of Pearson's Correlation Coefficient

The Pearson product-moment correlation coefficient was used to calculate the correlation between the various micro-parameters and macro-parameters; the results are shown in Table 5.

Table 5. Results of pearson correlation coefficient calculations.

No.	E/GPa	ν	σ_c/MPa	$FCR/(\text{°}/\text{MPa})$	σ_{ci}/MPa	σ_{cd}/MPa
E^*	0.645556	0.480193	0.071099	0.139484	0.087542	0.009629
k^*	−0.068016	0.334814	−0.077857	0.047656	−0.068842	−0.073569
$\bar{E}^*$	0.667735	−0.449355	0.018203	0.038409	0.027317	−0.046789
$\bar{k}^*$	−0.163237	0.616762	−0.19203	−0.078364	−0.177102	−0.112986
$\bar{\sigma}_c$	0.069494	−0.022027	0.748206	−0.687839	0.747732	0.715982
$\bar{c}$	−0.094335	0.000001	−0.060285	0.05267	−0.065542	0.016549
$\bar{\varphi}$	−0.007097	0.022027	−0.028295	0.364242	−0.030434	0.018956
μ	0.01449	−0.164183	−0.264745	−0.078028	−0.247873	−0.2232
β	−0.039331	0.061676	−0.246729	0.180937	−0.260794	−0.191069
R_f	0.278568	−0.167407	0.494899	−0.247313	0.491796	0.573658

The results of the Pearson correlation coefficient calculations are presented in a bar chart, as shown in Figure 3.

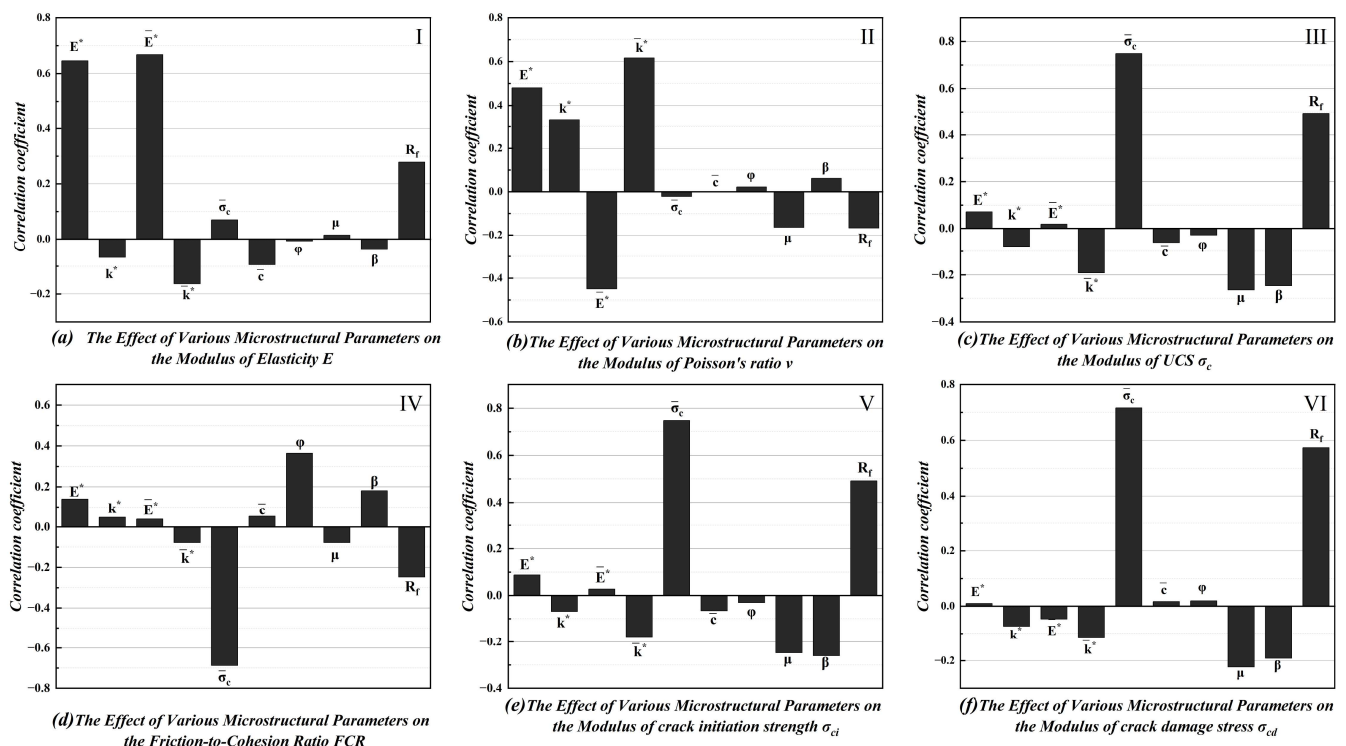


Figure 3. Results of Pearson correlation coefficient calculations: (a) The Effect of Various Microstructural Parameters on the Modulus of Elasticity E ; (b) The Effect of Various Microstructural Parameters on the Modulus of Poisson's ratio ν ; (c) The Effect of Various Microstructural Parameters on the Modulus of UCS σ_c ; (d) The Effect of Various Microstructural Parameters on the Friction-to-Cohesion Ratio FCR; (e) The Effect of Various Microstructural Parameters on the Modulus of crack initiation strength σ_{ci} ; (f) The Effect of Various Microstructural Parameters on the Modulus of crack damage stress σ_{cd} .

Based on Figure 3, the primary influencing factors for each macro-parameter can be preliminarily identified, as analysed below:

- (1) As can be seen from Figure 3a, E^* , $\bar{E}^*$ and R_f have a significant influence on the elastic modulus E ; $\bar{k}^*$ has a relatively large influence on E ; the influence of the remaining micro-parameters on the elastic modulus E is negligible. Therefore, it is preliminarily concluded that the elastic modulus E is primarily governed by E^* , $\bar{E}^*$, R_f and $\bar{k}^*$;
- (2) As shown in Figure 3b, E^* , k^* , $\bar{E}^*$ and $\bar{k}^*$ have a significant and pronounced effect on the Poisson's ratio ν . Consequently, it is preliminarily concluded that the Poisson's ratio ν is primarily governed by E^* , k^* , $\bar{E}^*$ and $\bar{k}^*$;
- (3) As shown in Figure 3c, $\bar{\sigma}_c$ and R_f have a significant influence on the uniaxial compressive strength σ_c , whilst μ and β have a greater influence on σ_c . The influence of the remaining microstructural parameters on the uniaxial compressive strength σ_c is negligible; therefore, it is preliminarily concluded that the uniaxial compressive strength σ_c is primarily governed by $\bar{\sigma}_c$, R_f , μ and β ;
- (4) As shown in Figure 3d, $\bar{\sigma}_c$, $\bar{\varphi}$, and R_f have a significant influence on the cohesion ratio FCR , whilst β and $\bar{E}^*$ have a relatively large influence on FCR ; the influence of the remaining micro-parameters on the cohesion ratio FCR is negligible. Therefore, it is preliminarily concluded that the cohesion ratio FCR is primarily governed by $\bar{\sigma}_c$, $\bar{\varphi}$, R_f , β , and $\bar{E}^*$;
- (5) As shown in Figure 3e, $\bar{\sigma}_c$ and R_f have a significant influence on the crack initiation strength σ_{ci} , whilst μ and β have a considerable influence on σ_{ci} . The influence of the remaining microstructural parameters on the crack initiation strength σ_{ci} is negligible. Therefore, it is preliminarily concluded that the crack initiation strength σ_{ci} is primarily governed by $\bar{\sigma}_c$, R_f , μ and β ;
- (6) As shown in Figure 3f, $\bar{\sigma}_c$ and R_f have a significant influence on the crack damage stress σ_{cd} , whilst μ and β have a considerable influence on σ_{cd} . The influence of the remaining microstructural parameters on the crack damage stress σ_{cd} is negligible. Therefore, it is preliminarily concluded that the crack damage stress σ_{cd} is primarily governed by the combined effects of $\bar{\sigma}_c$, R_f , μ and β .

Following the Pearson correlation analysis, a stepwise validation framework combining multivariate analysis of variance (ANOVA) and multiple regression analysis was adopted, with the aim of systematically identifying the influence mechanisms of micro-parameters on macro-responses at the statistical level and quantifying the extent of their effects. Specifically, micro-parameters with a linear correlation to the macro-response were first preliminarily screened via Pearson correlation analysis to establish a candidate set of influencing factors; subsequently, multivariate analysis of variance was introduced to test the independent main effects of each micro-parameter whilst controlling for other variables, thereby eliminating spurious correlations caused by multicollinearity among parameters and verifying the robustness of the Pearson analysis results; thereafter, based on multiple regression models, the direction of effects and contribution levels of each significant parameter were further analysed, ultimately forming a comprehensive understanding of the sensitivity levels of micro-parameters.

The rationale for this integrated validation strategy lies in the complementary roles of these three methods in statistical inference. As an exploratory tool, Pearson correlation analysis excels at rapidly identifying linear trends between two variables, but it cannot address the issue of confounding effects in scenarios involving multiple parameters; multivariate analysis of variance, through the decomposition of Type III sum of squares, can isolate the net effects of individual parameters whilst controlling for other factors, thereby effectively identifying independent sources of influence; multiple regression analysis, building upon

the confirmation of significance, quantifies the strength of effects using metrics such as standardised regression coefficients or partial Eta-squared, thereby facilitating a leap in inference from the mere presence of an effect to its specific magnitude. The progressive combination of these three methods not only avoids the biased conclusions that a single method might yield but also aligns with the logical sequence of ‘screening first, validation next, and quantification last’ in PFC parameter calibration research.

However, the essential characteristic of PFC numerical simulation is that, given the same combination of microscopic parameter inputs, the macroscopic response output is deterministic—that is, repeating the same set of parameter settings will not produce any variation. This represents a fundamental difference from the nature of physical experiments, which involve random errors. Consequently, this study did not employ traditional repeated experiments but instead utilised an orthogonal design to arrange multi-parameter combination tests. This resulted in the degrees of freedom for error terms depending primarily on the structure of the experimental design itself rather than on repeated measurements; when the number of independent variables is high, this can easily lead to a situation where the degrees of freedom are insufficient. This limitation has a certain impact on the statistical power of the F-test, meaning that for parameter relationships that are genuinely present but have moderate effect sizes, the test may tend to be conservative. To mitigate this issue, this study simultaneously outputs partial Eta-squared as an effect size measure in the IBM SPSS Statistics v22.0 analysis. This measure uses the total variance of the dependent variable as a reference frame, reflecting the proportion of variance explained by a particular parameter after controlling for other factors. Its calculation is not directly constrained by degrees of freedom, and thus provides a more robust assessment of effects in small-sample or low-degrees-of-freedom scenarios. Furthermore, the magnitude of the partial Eta-squared can be interpreted according to the effect size criteria proposed by Cohen, thereby providing an auxiliary basis for ranking the importance of parameters that is independent of significance testing. To further enhance the reliability of the conclusions, this study focused on the magnitude of changes in adjusted R^2 and the stability of standardised regression coefficients during the multiple regression analysis stage. By cross-validating the predictive accuracy of the regression models, the robustness of the significance conclusions in the multivariate analysis of variance was indirectly corroborated.

5.2.2. Multivariate Analysis of Variance

In assessing parameter sensitivity, a dual verification approach combining significance tests and effect size metrics can be employed. Regarding the significance level, $p < 0.05$ is adopted as the basic threshold, whilst $p < 0.01$ is considered highly significant. Concurrently, the partial η^2 is introduced to measure the strength of the independent effects of each micro-parameter, thereby compensating for the constraints on the power of the F-test imposed by the low degrees of freedom in the multivariate analysis of variance. Specifically, when a parameter satisfies $p < 0.05$, it is judged to have a practically significant influence on the macro-response and is denoted as “*”; where $p < 0.01$, it is judged to have a significant influence, denoted as “**”. Furthermore, due to the aforementioned issue of model degrees of freedom, after comprehensive analysis, a bias η^2 of 0.45 was selected as the basic threshold; that is, regardless of whether a parameter is classified as having a substantial or significant influence, its bias η^2 must exceed 0.45 to compensate for potential misjudgements of p -values resulting from insufficient model degrees of freedom. Subsequently, to ensure the statistical robustness and engineering interpretability of the parameter sensitivity ranking, the results were corroborated using standardised regression coefficients from multiple regression analysis and model cross-validation. The corresponding statistical parameters for each factor and test indicator are listed in Table 6.

Table 6. Results of multifactorial analysis of variance.

<i>Factors</i>	<i>E</i>			<i>ν</i>			<i>σ_c</i>			<i>FCR</i>			<i>σ_{ci}</i>			<i>σ_{cd}</i>		
<i>Statistical Parameters</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>	<i>F</i>	<i>p</i>	<i>Sig.</i>
<i>E</i> *	396.979	0.000	0.992	83.953	0.000	0.965	1.369	0.324	0.313	7.307	0.025	0.709	0.080	0.925	0.026	1.824	0.240	0.378
<i>k</i> *	4.481	0.064	0.599	43.860	0.000	0.936	0.801	0.492	0.211	0.164	0.852	0.052	0.532	0.613	0.151	0.641	0.559	0.176
<i>E</i> *	419.230	0.000	0.993	75.626	0.000	0.962	1.059	0.404	0.261	0.116	0.893	0.037	0.230	0.801	0.071	1.168	0.373	0.280
<i>k</i> *	25.528	0.001	0.895	141.907	0.000	0.979	5.109	0.051	0.630	1.854	0.236	0.382	1.000	0.422	0.250	4.381	0.067	0.594
<i>σ_c</i>	4.863	0.056	0.618	0.178	0.842	0.056	59.188	0.000	0.952	37.189	0.000	0.925	24.014	0.001	0.889	59.248	0.000	0.952
<i>c</i>	9.490	0.014	0.760	0.009	0.991	0.003	0.439	0.664	0.128	5.073	0.051	0.628	0.122	0.887	0.039	0.512	0.623	0.146
<i>φ</i>	0.049	0.952	0.016	0.290	0.758	0.088	0.617	0.571	0.171	10.316	0.011	0.775	0.032	0.968	0.011	0.540	0.609	0.152
<i>μ</i>	0.263	0.777	0.081	0.682	0.541	0.185	1.153	0.377	0.278	1.202	0.364	0.286	0.395	0.690	0.116	1.130	0.383	0.274
<i>β</i>	2.217	0.190	0.425	1.523	0.292	0.337	6.768	0.029	0.693	2.481	0.164	0.453	1.912	0.228	0.389	7.568	0.023	0.716
<i>R_f</i>	73.462	0.000	0.961	10.131	0.012	0.772	26.161	0.001	0.897	5.571	0.043	0.650	15.363	0.004	0.837	25.927	0.001	0.896

To analyse the extent of the influence of experimental factors on the experimental indicators more intuitively, the results of the analysis of variance were plotted as a bar chart. To ensure the simplicity of the legend, only the F-statistic is shown, as shown in Figure 4.

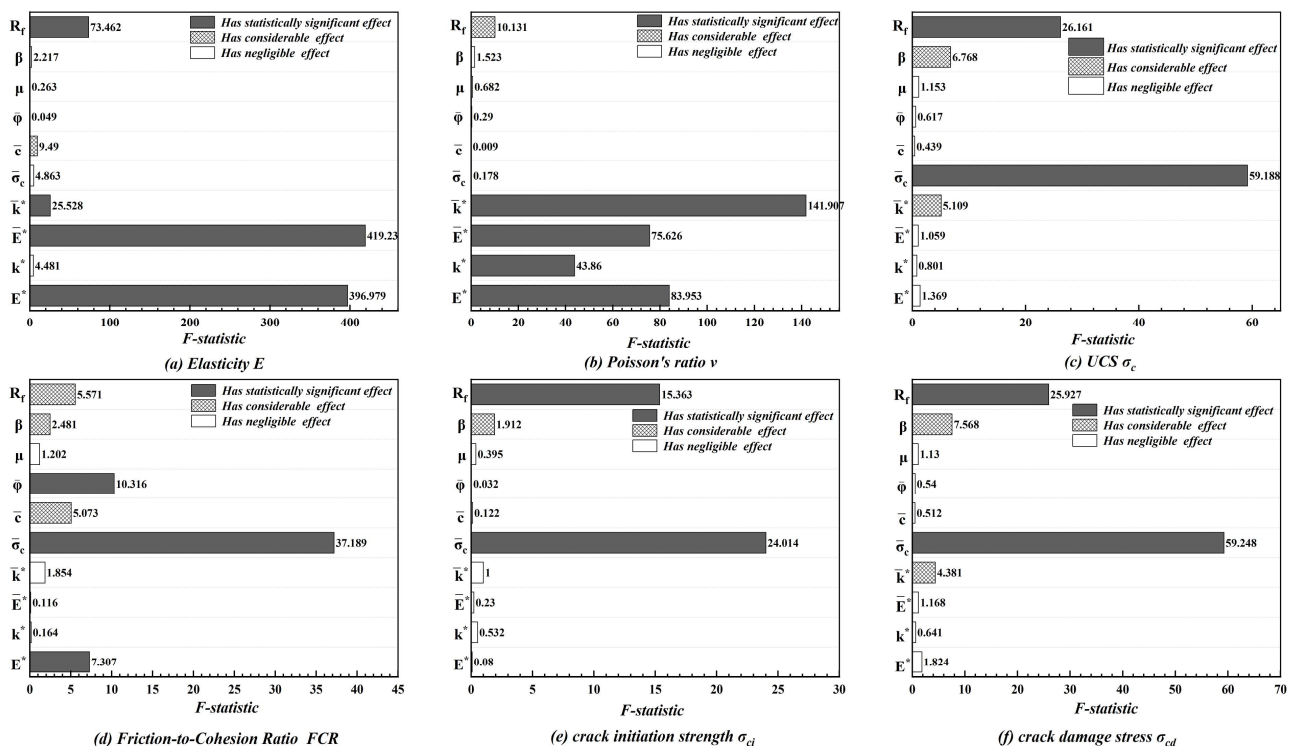


Figure 4. F-statistic for multi-factor analysis of variance: (a) F-statistic of each micro-parameter on Elasticity E ; (b) F-statistic of each micro-parameter on Poisson's ratio ν ; (c) F-statistic of each micro-parameter on UCS σ_c ; (d) F-statistic of each micro-parameter on Friction-to-Cohesion Ratio FCR; (e) F-statistic of each micro-parameter on crack initiation strength σ_{ci} ; (f) F-statistic of each micro-parameter on crack damage stress σ_{cd} .

Combining the information presented in Figures 3 and 4, and synthesising the specific results of the Pearson correlation analysis and the multi-factor analysis of variance, the relationship between the selected micro-parameters and macro-parameters is further explained as follows:

- (1) Figures 3a and 4a both demonstrate that E^* , $\bar{E}^*$, $\bar{k}^*$, and R_f have a significant influence on the elastic modulus E . Figure 4a further shows that $\bar{c}$ also has a considerable influence on the elastic modulus E . Furthermore, based on significance tests and the η^2 test, it has been established that $\bar{c}$ is also a major influencing factor on the elastic modulus E . Consequently, it is concluded that E^* , $\bar{E}^*$, $\bar{k}^*$, and R_f exert a dominant influence on the elastic modulus E ;
- (2) In Figures 3b and 4b, it is evident that E^* , k^* , $\bar{E}^*$ and $\bar{k}^*$ have a significant influence on the Poisson's ratio ν . It is also shown that R_f has a considerable influence on the Poisson's ratio ν ; however, following a significance test for R_f and a bias test for η^2 , it is concluded that R_f is also a major influencing factor on the Poisson's ratio ν . Consequently, it is considered that E^* , k^* , $\bar{E}^*$, $\bar{k}^*$, and R_f exert a dominant influence on the Poisson's ratio ν ;
- (3) In Figure 3c, calculations of the Pearson correlation coefficients indicate that $\bar{\sigma}_c$ and R_f have a significant effect on the uniaxial compressive strength σ_c , and that $\bar{k}^*$, μ and β have a substantial effect on it; in Figure 4c, the multi-factor analysis of variance also reveals that $\bar{\sigma}_c$, R_f , $\bar{k}^*$, μ , β have a significant effect on the uniaxial compressive

- strength σ_c . Taking all the above considerations into account, it is concluded that $\bar{\sigma}_c$, R_f , $\bar{k}^*$, μ , and β exert a dominant influence on the uniaxial compressive strength σ_c ;
- (4) As indicated by the Pearson correlation coefficients, $\bar{E}^*$, $\bar{\sigma}_c$, $\bar{\varphi}$, β and R_f have a significant effect on the cohesion ratio FCR ; however, the values obtained from the multi-factor analysis of variance and the bar charts show that $\bar{\sigma}_c$, β and R_f do indeed have a significant effect on the cohesion ratio FCR ; however, the effects of $\bar{E}^*$ do not meet the criteria for significance, as neither the p -value nor the bias η^2 satisfy the required thresholds. Meanwhile, $\bar{c}$ has a p -value of 0.051, which is slightly higher than the threshold of 0.05, and its bias η^2 exceeds the threshold of 0.45. Therefore, it is concluded that $\bar{c}$ also has a significant effect on the cohesion ratio FCR . Based on the above analysis, $\bar{\sigma}_c$, $\bar{c}$, $\bar{\varphi}$, β , and R_f have a dominant influence on the cohesion ratio FCR ;
 - (5) As indicated by the Pearson correlation coefficients, $\bar{\sigma}_c$, R_f , β and μ have a significant influence on the crack initiation stress σ_{ci} ; however, the values obtained from the multi-factor analysis of variance and the bar charts show that $\bar{\sigma}_c$ and R_f have a significant influence on the crack initiation stress σ_{ci} . The influences of β and μ do not meet the criteria for significance, as neither the p -values nor the η^2 satisfy the criteria for significance. Therefore, it is concluded that $\bar{\sigma}_c$ and R_f have a dominant influence on the crack initiation stress σ_{ci} ;
 - (6) With regard to the crack damage stress σ_{cd} , the Pearson correlation coefficient test indicates that $\bar{\sigma}_c$, R_f , β and μ have a significant influence on the crack damage stress σ_{cd} . However, the statistical parameters obtained from the multivariate analysis of variance show that the contribution of μ to the crack damage stress does not meet the criteria for significance, and it was found that the contribution of $\bar{k}^*$ is clearly predominant. Based on the above analysis, $\bar{\sigma}_c$, R_f , β and $\bar{k}^*$ have a dominant influence on the crack damage stress σ_{cd} ;
 - (7) Regression analysis of the significant influencing factors and test parameters yields the following relationship between macro- and micro-scale parameters:

$$E = -0.764 + 1.213 \times E^* + 1.254 \times \bar{E}^* - 0.307 \times \bar{k}^* - 0.177 \times \bar{c} + 0.523 \times R_f \quad (R^2 = 0.970). \quad (6)$$

$$\nu = 0.150 + 0.061 \times E^* + 0.042 \times k^* - 0.057 \times \bar{E}^* + 0.078 \times \bar{k}^* - 0.021 \times R_f \quad (R^2 = 0.942). \quad (7)$$

$$\sigma_c = 2.649 - 1.184 \times \bar{k}^* + 4.613 \times \bar{\sigma}_c - 1.521 \times \beta + 3.051 \times R_f \quad (R^2 = 0.885). \quad (8)$$

$$FCR = 17.564 + 1.431 \times E^* - 7.058 \times \bar{\sigma}_c + 3.736 \times \bar{\varphi} - 2.536 \times R_f + 1.857 \times \beta \quad (R^2 = 0.652). \quad (9)$$

The results of this linear regression analysis show that the model, with FCR as the dependent variable and the five PFC micro-parameters as independent variables, has an R^2 of 0.719 and an adjusted R^2 of 0.652, indicating that the model explains 65.2% of the variation in FCR . Although this R^2 value is considered above average in the field of engineering prediction, it remains relatively low compared to traditional calibration methods such as stress–strain curve fitting. This stems from the inherent multi-scale complexity of the PFC discrete element model: On the one hand, as a second-order derived parameter obtained by inverting the failure angle measurement using the Mohr–Coulomb equation, FCR inherently carries subjective errors in failure plane identification, uncertainties in the dynamic evolution of the post-peak fracture surface, and systematic biases arising from differences between uniaxial and triaxial stress states; on the other hand, the macroscopic mechanical response of granular materials is essentially determined by the non-linear

coupling of multiple parameters, such as particle contact stiffness, bond strength and friction coefficient. Linear regression models struggle to fully capture these complex interactive effects; furthermore, the relatively limited sample size of the model further restricts its ability to identify higher-order and interaction terms. However, it is worth emphasising that this R^2 value is significantly superior to the regression results obtained using equivalent cohesion or equivalent internal friction angle as independent variables alone (according to preliminary explorations in this study, the highest R^2 for either of these was only around 0.3). This comparison precisely demonstrates the methodological advantage of the *FCR* approach: Cohesion and the internal friction angle exhibit strong non-linear coupling under the regulation of PFC microstructural parameters; different combinations of microstructural parameters may yield similar absolute values of (c, φ) yet result in distinctly different *FCR* values, causing the individual information to be obscured by the ‘noise’ of parameter interactions when analysed in isolation; In contrast, by reducing the two-dimensional coupled parameters to a comprehensive indicator reflecting the strength mechanism, *FCR* effectively isolates the synergistic fluctuations of c and φ , amplifying the regulatory signals of micro-parameters on the material’s brittle tensile and shear slip failure modes, thereby achieving greater explanatory power within the same linear framework. Therefore, although the adjusted R^2 of 0.652 has not yet reached the ideal predictive accuracy, in highly non-linear, significantly stochastic discrete systems such as PFC, this model can reveal the regulatory patterns of micro-parameters on the macroscopic strength constitutive mechanism.

$$\sigma_{ci} = -2.883 + 2.644 \times \bar{\sigma}_c + 2.118 \times R_f \quad (R^2 = 0.829). \quad (10)$$

$$\sigma_{cd} = 2.653 + 4.532 \times \bar{\sigma}_c + 2.981 \times R_f - 1.581 \times \beta - 1.073 \times \bar{k}^* \quad (R^2 = 0.882). \quad (11)$$

6. Discussion

This paper focuses on the calibration of macro- and micro-parameters for the PFC^{2D} parallel bonding model. Based on an orthogonal experimental design, it systematically analyses the influence of 10 micro-parameters on 6 macro-mechanical indicators, and innovatively proposes the Friction Coefficient Ratio (*FCR*) as an indicator to address the problem of strong coupling between cohesion and the angle of internal friction. The following discussion covers both the innovative contributions and the limitations of this work.

(1) Proposal of the comprehensive Cohesion Ratio (*FCR*) indicator to achieve dimensionality reduction and decoupling of strength parameters. Addressing the non-linear coupling and multi-solution dilemma between cohesion c and internal friction angle φ in PFC parameter calibration, this paper innovatively proposes the Cohesion Ratio $FCR = \varphi^*/c^*$, reducing the two-dimensional strength parameter space to one dimension. Under the constraint of uniaxial compressive strength, this indicator establishes a one-to-one correspondence with (c, φ) combinations, effectively decoupling their synergistic fluctuation effects. Consequently, the explanatory power of the regression model (adjusted $R^2 = 0.652$) is significantly superior to that of calibrating c or φ individually ($R^2 \approx 0.3$), providing a new tool for discrete element parameter calibration that combines both physical significance and statistical robustness.

(2) Establishing a progressive statistical validation framework and introducing the partial Eta-squared effect measure. This paper establishes a three-tier progressive system comprising ‘Pearson correlation analysis—multifactor analysis of variance—multivariate regression analysis’, thereby realising a complete chain of inference from factor screening and significance verification to effect quantification. To address the limitation of insufficient degrees of freedom in orthogonal designs caused by the deterministic nature of

PFC simulations, partial Eta-squared is introduced as an auxiliary effect size metric. Its calculation is not constrained by degrees of freedom and can provide a robust ranking of parameter importance in small-sample scenarios, thereby compensating for the low power of traditional F-tests.

(3) Equivalent extraction of shear strength parameters is achieved within a uniaxial compression framework. Overcoming the limitation of traditional methods requiring additional triaxial simulations, the failure angle β is measured from the macroscopic fracture surface morphology following peak stress. Based on Mohr–Coulomb theory, the equivalent internal friction angle and cohesion are calculated retrospectively, thereby integrating the calibration of shear strength parameters into the uniaxial testing framework. This establishes a theoretical bridge between uniaxial simulation and shear strength parameters whilst reducing computational costs.

However, the study still has several methodological and modelling issues that warrant further discussion.

(4) The predictive accuracy of the *FCR* regression model requires improvement. Although the explanatory power of the *FCR* model surpasses that of traditional methods, the adjusted R^2 of 0.652 has not yet reached an ideal predictive level. This stems from the fact that, as a secondary derivative parameter derived from the measurement of the failure angle and theoretical inversion, the *FCR* carries systematic biases such as subjective errors in failure plane identification and differences in uniaxial/triaxial boundary conditions, further compounded by the fact that linear models struggle to fully capture the multi-parameter non-linear coupling effects in granular materials, whilst the limited sample size also restricts the ability to identify higher-order terms. Future work could consider introducing non-linear regression or machine learning methods to enhance model accuracy.

(5) The subjectivity of failure angle measurements and the discretisation limitations of orthogonal design. *FCR* extraction relies on manual judgement based on the dip angle of the fracture plane; local variations and dynamic evolution can easily introduce measurement errors. At the same time, a three-level orthogonal design may result in the omission of optimal parameter combinations, and the excessive number of factors leads to a low degree of freedom for errors, causing the F-test to be overly conservative. In the future, it will be necessary to develop automatic fracture plane recognition algorithms and combine them with response surface methods or uniform designs to increase the sampling density in the parameter space.

(6) The applicability of the uniaxial stress state requires further validation. The derivation of the *FCR* is based on the Mohr–Coulomb criterion and the assumption of uniaxial conditions, whereas rock masses in practice are often subjected to triaxial stress states; the boundary condition of zero lateral stress may introduce systematic bias. Subsequent work should validate the applicability of the *FCR* method through triaxial compression simulations and explore the evolutionary patterns of strength parameter composition mechanisms under complex stress paths.

7. Conclusions

This paper takes the PFC^{2D} parallel bonding model as its subject of study. Based on uniaxial compression numerical experiments and orthogonal experimental design, a systematic sensitivity analysis of macro- and micro-parameters was conducted, and the comprehensive indicator ‘Friction-to-Cohesion Ratio (*FCR*)’ was innovatively proposed. The main conclusions are as follows:

(1) The influence of microstructural parameters on macroscopic mechanical responses exhibits significant parameter specificity and variations in indicators. The elastic modulus E is primarily governed by the effective elastic modulus of the particles E^* , the effective elastic

modulus of parallel bonding $\bar{E}^*$, the tangential stiffness ratio of parallel bonding $\bar{k}^*$, and the filler ratio R_f ; the Poisson's ratio ν is mainly influenced by E^* , the tangential stiffness ratio of the particles k^* , $\bar{E}^*$, $\bar{k}^*$, and R_f ; uniaxial compressive strength σ_c , crack initiation strength σ_{ci} and crack damage stress σ_{cd} are primarily regulated by the parallel bonding tensile strength $\bar{\sigma}_c$ and R_f , whilst the particle surface friction coefficient μ and the moment distribution coefficient β also exert a significant influence on these strength parameters. The above patterns reveal the fundamental characteristic that elastic parameters and strength parameters in the PFC model are governed by different microscopic mechanisms, providing a theoretical basis for a phased, target-oriented parameter calibration strategy.

(2) The introduction of the cohesion ratio (*FCR*) has effectively resolved the issue of strong coupling between cohesion and the angle of internal friction in parameter sensitivity analysis. Traditional methods treat c and φ as independent parameters for separate examination; however, under the control of the PFC microstructural parameters, there exists a significant non-linear synergistic effect between the two—different (c, φ) combinations may yield similar uniaxial compressive strengths, leading to a dilemma of high-dimensional coupling and multiple solutions in parameter inversion. The *FCR* is defined as the ratio of the equivalent angle of internal friction to the equivalent cohesion ($FCR = \varphi^*/c^*$). By reducing the two-dimensional strength parameter space to one dimension, it effectively decouples the synergistic fluctuations of c and φ , amplifying the regulatory signals of the microscopic parameters on the brittle tensile and shear slip failure modes of the material. Linear regression analysis indicates that the model with *FCR* as the dependent variable achieves an R^2 of 0.652, significantly outperforming regression results using c or φ alone (with a maximum R^2 of only 0.31), thereby validating the superiority of *FCR* in enhancing the interpretability of parameter sensitivity analysis. Furthermore, this parameter is derived from the uniaxial strength expression based on the Mohr–Coulomb criterion and maintains a one-to-one correspondence with the (c, φ) combination under the constraint of uniaxial compressive strength, ensuring the uniqueness of the parameter inversion; simultaneously, the introduction of *FCR* transforms macro–micro parameter sensitivity analysis from the traditional approach of examining the effects of c and φ on the macroscopic response separately to a systematic revelation of the intrinsic mechanisms by which micro-parameters regulate the composition of material strength, significantly enhancing the efficiency and physical interpretability of parameter calibration.

(3) The method for inverting shear strength parameters based on uniaxial compression simulations and Mohr–Coulomb theory has demonstrated feasibility and defined applicability limits. By tracking the morphology of the specimen's macroscopic fracture surface following peak stress, precisely measuring the failure angle β , calculating the equivalent internal friction angle based on $\varphi = 90^\circ - 2\beta$, and then substituting this into the uniaxial compressive strength formula to determine the equivalent cohesion, shear strength parameters can be extracted without increasing the computational cost of triaxial simulations. The uncertainty of this method primarily stems from the subjectivity of the failure angle measurement, the dynamic evolution of the fracture surface after peak stress, and the boundary differences between uniaxial and triaxial stress states. It is necessary to reduce variability through statistical averaging across multiple specimens and to clearly define the obtained parameters as macroscopic equivalent values for the aggregate of particles rather than true rock physical constants.

(4) A progressive validation framework comprising Pearson correlation analysis, multivariate analysis of variance (ANOVA) and multiple regression analysis was established. Through dual assessment using significance tests and the partial η^2 effect size metric, the independent main effects of each micro-parameter on the macro-response and their contribution levels were systematically identified, effectively overcoming the issue of low

degrees of freedom in PFC numerical simulations caused by a lack of repeated experiments. This analytical framework combines statistical robustness with engineering interpretability, providing a methodological reference for research into the calibration of PFC macro- and micro-parameters.

Therefore, based on the principle of ‘independent parameters first, coupled parameters second; elasticity first, strength second’, the parameter calibration sequence is determined as follows, with the specific process shown in Figure 5.

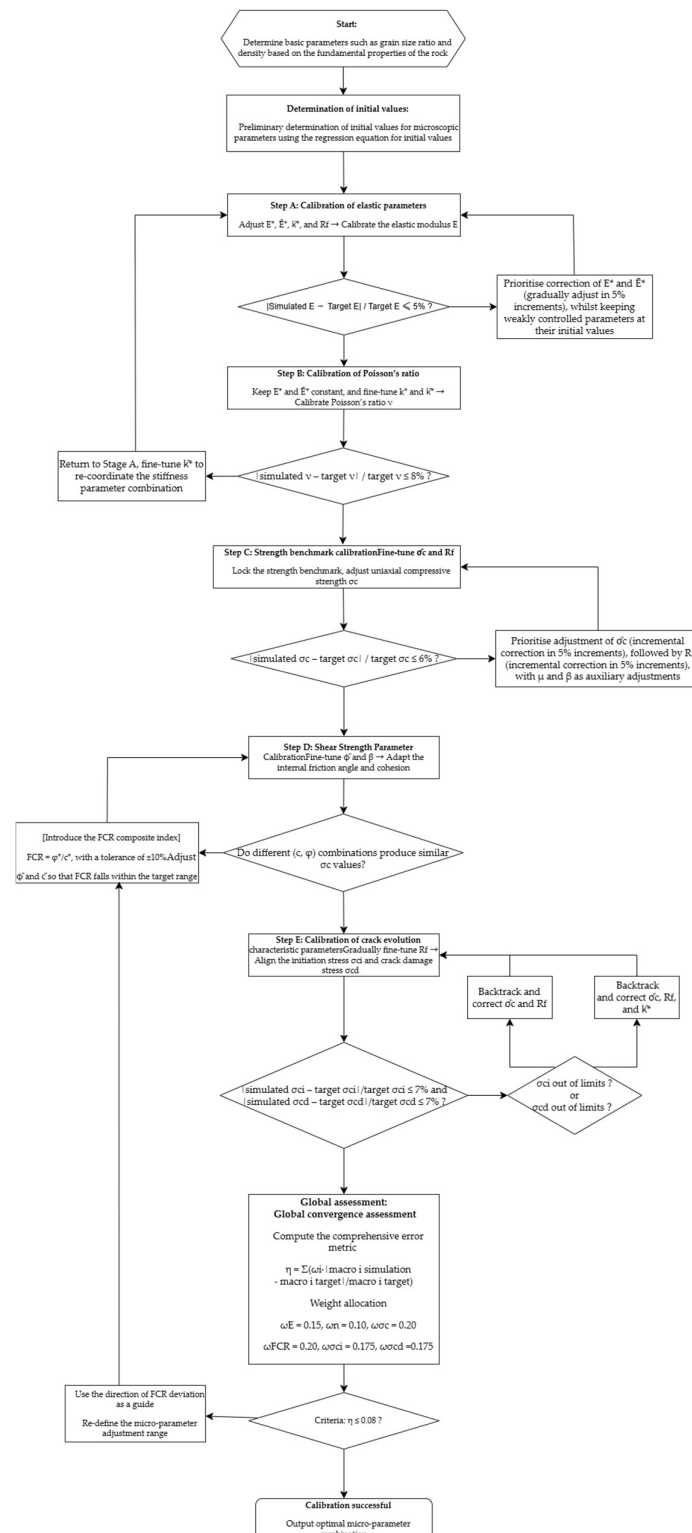


Figure 5. Micro-parameter calibration process.

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