Quantitative Determination Approach of Rock Micro Tensile Strength Based on Particle Flow Code

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Abstract. Rock Particle Flow Code (PFC) model has numerous micro parameters, and its quantitative determination is completed by try and error, which consumes a large amount of time and efforts of researchers. Under this background, the quantitative determination approach of rock micro parameters is of significant importance. This study proposes a simplified model based on PFC^{2D} to analyze the stress mechanism from the perspectives of force balance and deformation equilibrium, and explores the theoretical relation between macro tensile strength and micro parameters. The direct tensile test is simulated by PFC^{2D} to explore the influence of contact normal bond strength (micro tensile strength) σ_{cn}, particle size (maximum particle diameter D_{max}, and particle diameter ratio D_{max}/D_{min}) and normal to shear stiffness ratio k_n/k_s on macro tensile strength. Based on the results of theoretical analysis and statistical analysis, the quantitative determination approach of micro tensile strength in direct tension test is determined.

Keywords: Particle Flow Code (PFC) · Contact Bond Model (CBM) · Tensile strength · Particle size · Stiffness ratio

1 Introduction

In 2004, the Particle Flow Code (PFC) model suitable for rock materials, namely, Bonded Particle Model (BPM), was proposed by Potyondy and Cundall [1]. At present, there are two kinds of Bonded Particle Model that can be used to simulate rock micro characteristics including Contact Bond Model (CBM) and Parallel Bond Model (PBM). As a simplification of PBM, CBM has 5 micro parameters of control strength and stiffness, while PBM has 7 micro parameters. Since the micro parameters of rock PFC model cannot be directly obtained by experiment, its quantitative determination is completed by try and error [2], which consumes a large amount of time and efforts of

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researchers. Under this background, the quantitative determination approach of rock micro parameters is of significant importance.

Huang [3] (1999) studied the qualitative relations of micro parameters in CBM with the elasticity modulus E, Poisson's ratio v, uniaxial compressive strength σ_c and fracture toughness by the dimensional analysis and simulation of uniaxial and biaxial compressive tests. Yang et al. [4] (2006) obtained the expressions for dimensionless quantitative relations of σ_c, E and v with the micro parameters by statistical analysis and simulation of uniaxial compression tests. Jeoungseok [5] (2007) used the Plackett-Burman (PB) test and Central Composite Design (CCD) to obtain micro parameters that can preferably simulate the specimens. Although Yoon derived a rather complete method for selecting CBM micro parameters, it had cumbersome procedure and was thus not easily applicable. The above scholars studied the relationship between macro response and micro parameters of rock either qualitatively or quantitatively, and applied their results to the calibration of micro parameters.

However, there were the following two problems: a. Due to the large number of micro parameters, substantial numerical tests were required to obtain the statistical relation expression for macro and micro parameters within a limited range. b. Due to the limited research range of micro parameter in numerical tests, the application of the quantitative relation of macro and micro parameters is limited. Therefore, the study of intrinsic relation between macro and micro parameters through theoretical analysis is of great significance to reducing the number of numerical tests and expanding the application range.

This paper studies the relationship between macro tensile strength and micro parameters in CBM by direct tensile tests. A simplified theoretical model is proposed to analyze the theoretical relation between macro tensile strength and micro parameters. Through a large number of numerical tests, the quantitative relationship between macro tensile strength and micro parameters of rock material was obtained, and the above theoretical formula was verified and modified. Finally, a approach with less numerical tests for determining the micro tensile strength is presented.

2 Mechanical Analysis of Theoretical Model for Direct Tensile Test

The dissimilarity of simulation objects, the pattern of particle diameter distribution (mean distribution, Gaussian distribution) and the randomness of particle spatial distribution lead to tremendous difference in micro geometrical characteristics (diameter and spatial location of particles filling the numerical specimens) between numerical specimens, thereby increasing the difficulty of studying the mechanical properties of rock PFC model through theoretical analysis. This paper puts forward a theoretical model of regular arrangement to study the theoretical relationship between macro tensile strength and micro parameters. The theoretical model presented in Fig. 1 consists of particles with two particle sizes arranged in a reciprocal layer, and the particle diameters are d_1 and d_2 (radius are r_1, r_2). The included angle between horizontal line and the line between the centers of two adjacent particles is θ ($0° < \theta < 90°$), as shown in Fig. 1. The coordination number [6] refers to the average number of contacts of per particle in a particle system. In the numerical specimens herein, the coordination number is 3.55–4.97. The closer the particle diameter ratio is to 1, the larger the coordination number. The coordination number of the theoretical model is 4, which is consistent with the numerical specimens. The mechanical characteristics of the theoretical model can be discussed through analyzing representative element (shown as the shadow areas in Fig. 1). The lengths in vertical and horizontal directions are l_1 and l_2, respectively. Sun et al. [6] defined $\alpha = \arctan(l_1/l_2)$ as the parameters describing the geometrical characteristics of periodic structures. As shown in Fig. 1, $\alpha = \theta$. In this paper, call α periodic structure geometric characteristic angle (geometric characteristic angle for short).

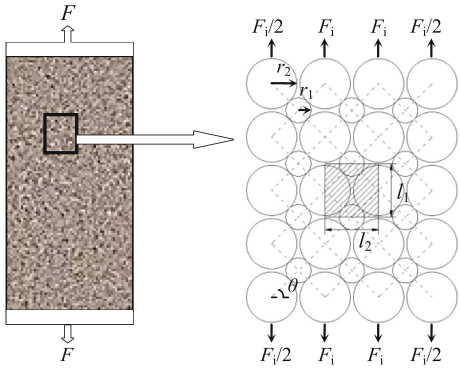


Fig. 1. Theoretical model.

The width of the theoretical model is L, and there are n particles with the particle size of d_2. The tension forces on the two sides of the model are F. Then, the macro tensile strength can be represented as Formula (1).

$$\sigma_t = \frac{F}{L} = \frac{(n-1)F_i}{(n-1)l_2 + d_2} = \frac{F_i}{(d_1 + d_2)\cos\theta + d_2/(n-1)} \quad (1)$$

In Fig. 2, the stress states on both sides of particle O_{A1} are symmetrical, $F_i = 2(f_n \sin\theta + f_s \cos\theta)$. After a micro deformation, O_{A1} and O_{B1} move to the positions of O_{A2} and O_{B2}, and geometric characteristic angle changes from θ to β, as presented in Fig. 2. Let Δ_1 be the vertical displacement of O_{A1}, and Δ_2 is the horizontal position of O_{B1}, Δ_n is the normal deformation at contact point, Δ_s is the tangential deformation at contact point. According to force-displacement criterion of CBM, $f_n = k_n\Delta_n$, $f_s = k_s\Delta_s$. Δ_1 and Δ_2 can be represented as Formula (2). β can be expressed as Formula (3). The deformation of particles is very small. Let $\tan\beta = \tan\theta$, and the relation between normal deformation and tangential deformation is presented in Formula (4). The relation

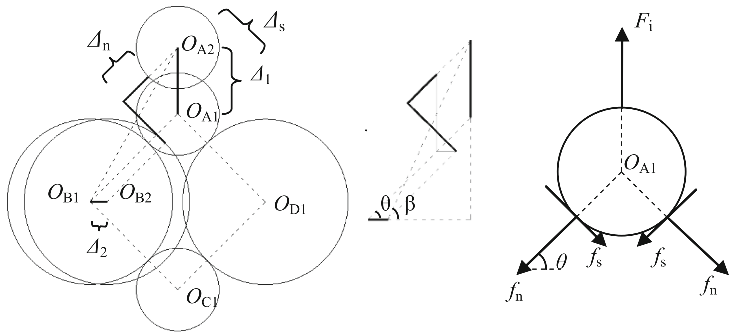


Fig. 2. Force analysis diagram of the representative element and force diagram at O_{A1}.

between normal force and tangential force at contact point between O_{A2} and O_{B2} is obtained, as presented in Formula (5).

$$\Delta_1 = \Delta_s \cos\theta - \Delta_n \sin\theta, \Delta_2 = \Delta_s \sin\theta - \Delta_n \cos\theta \quad (2)$$

$$\tan\beta = ((r_1 + r_2)\sin\theta + \Delta_1)/((r_1 + r_2)\cos\theta - \Delta_2) \quad (3)$$

$$\Delta_s/\Delta_n = 2\sin\theta\cos\theta = \sin 2\theta \quad (4)$$

$$f_s = f_n \times \sin 2\theta/(k_n/k_s) \quad (5)$$

When the load reaches the peak intensity of numerical specimen, the normal contact stress σ_n reaches the contact normal bond strength σ_{cn}. The relation between normal contact force f_n and contact normal bond strength σ_{cn} is $f_n = \sigma_{cn} * d_1$. The theoretical relation between macro tensile strength and micro tensile strength, particle size and stiffness ratio can be obtained, as shown in Formula (6). In this paper, $d_2 > d_1$, let $d_2 = d_{max}$, $d_1 = d_{min}$. The ratio of macro tensile strength σ_t to micro tensile strength σ_{cn} is called the macro to micro tensile strength scale coefficient K (the scale coefficient K for short) as shown in Formula (7). When $d_1 > d_2$, the analytical procedure is the same as above, and the expression for the scale coefficient K is consistent with Formula (7).

$$\sigma_t = 2\sigma_{cn}\frac{1}{1 + d_2/d_1}(1 - \frac{d_2}{L})(\tan\theta + \frac{\sin 2\theta}{k_n/k_s}) \quad (6)$$

$$K = 2\frac{1}{1 + d_{max}/d_{min}}(1 - \frac{d_{max}}{L})(\tan\theta + \frac{\sin 2\theta}{k_n/k_s}) \quad (7)$$

Formula (7) preferably displays the influence of micro parameters on macro tensile strength, respectively. σ_t and σ_{cn} present a linear correlation through the origin; the greater the normal to shear stiffness ratio k_n/k_s, the less the scale coefficient K; the larger the geometric characteristic angle θ, the greater the scale coefficient K. In Formula (7), the three factors $1/(1 + d_{max}/d_{min})$, $1 - d_{max}/L$ and $\tan\theta + \sin 2\theta/(k_n/k_s)$ of the scale coefficient K can be regarded as the correction terms of micro parameters d_{max}/d_{min}, d_{max}, θ and k_n/k_s on K, respectively.

Particle diameter ratio d_{max}/d_{min} and maximum particle diameter d_{max} are unable to fully describe the discrepancy in micro geometrical characteristics between different numerical specimens. The geometric characteristic angle θ, a later manually defined parameter, compensates for this deficiency. In theoretical model, θ is connected with particle size. When $r_2 > r_1$, the range of θ is shown in formula (8). When $r_1 > r_2$, the range of θ is shown in Formula (9). According to Formula (8) and (9), $r_2/r_1 = 0 \sim 1 + \sqrt{2}$.

$$\arcsin(r_2/(r_1+r_2)) < \theta < \arccos(r_2/(r_1+r_2)) \tag{8}$$

$$\arcsin(r_1/(r_1+r_2)) < \theta < \arccos(r_2/(r_1+r_2)) \tag{9}$$

It is noteworthy that there are only two types of particle diameters (d_{min}, d_{max}) in the theoretical model. Comparatively, in the numerical specimens herein, the particle diameters are evenly distributed in the interval (D_{min}–D_{max}), and the geometrical parameters (D_{min}/D_{max}, D_{max}) are inconsistent with the geometric parameters (d_{min}/d_{max}, d_{max}) in Formula (7) in terms of physical meaning. Therefore, it is worth discussing in depth whether the geometrical parameters of the numerical specimens can be used directly in (7) for calculating the scale coefficient K and whether a single numerical specimen will correspond to more than one theoretical models.

3 Simulation Programme and Results of Direct Tensile Test

3.1 Simulation Programme

Seven independent parameters are required to establish a CBM, including particle size (minimum particle diameter D_{min}, particle diameter ratio D_{max}/D_{min}), strength parameters (friction coefficient μ, contact shear bond strength τ_{cn}, and contact normal bond strength σ_{cn}), and stiffness parameters (contact modulus E_c, normal to shear stiffness ratio k_n/k_s). In this paper, the D_{min}, D_{max}/D_{min}, and σ_{cn} is test variables. Parameters with fixed value are referenced to the micro parameters of quartz sandstone simulated by Fu [7], and the values of micro parameters can be found in Table 1. In accordance with the existing research results [8–13], when σ_{cn} is smaller than τ_{cn} and k_n/k_s is greater than 1, it is easier to obtain numerical specimens in accordance with the mechanical characteristics of rocks.

By referring to the requirements of International Society for Rock Mechanics (ISRM) [14] for macro specimen size and micro grain size of rock specimen in uniaxial compression test, the specimen size of the numerical model in direct tension test is 50 mm * 100 mm, and the maximum particle diameter is smaller than 50 mm/20 = 2.5 mm. The scheme of direct tensile numerical test is shown in Table 2, where 7 sets of D_{min} and 8 sets of D_{max}/D_{min} can form 36 combinations of particle diameters that meet the requirements. 5 numerical tests are performed on 36 numerical specimens whose particle size combination is marked as A. σ_{cn} is set to 1, 5, 15, 20 and

Table 1. Micro parameters of Contact Bond Model.

Microparameters (abbreviation & unit)		Invariant	Variables
Particle size	Minimum particle diameter (D_{min}) (mm)		7 levels 0.2, 0.3, 0.4, 0.6, 0.8, 1, 2
	Particle diameter ratio (D_{max}/D_{min})		8 levels 1.2, 1.67, 2, 3, 4, 5, 6, 7
Strength parameters	Contact normal bond strength (σ_{cn}) (Mpa)		5 levels 1, 5, 15, 20, 30
	Contact shear bond strength (τ_{cs}) (MPa)	50	
	Ball friction coefficient (μ)	1.7	
Stiffness parameters	Normal to shear stiffness ratio (k_n/k_s)		4 levels 1, 2, 3.5, 6
	Contact Modulus (E_c) (GPa)	10	

30 MPa, respectively, and k_n/k_s is 3.5. A total of 180 numerical tests are carried out. 9 numerical tests are performed on 21 numerical specimens whose particle size combination is marked as B. σ_{cn} is set to 1, 5 and 15 MPa, and k_n/k_s is set to 1, 2 and 6, respectively. A total of 189 numerical tests are carried out. (To reduce the number of tests, the levels of micro tensile strength can be decreased to 3 according to simulation results below.)

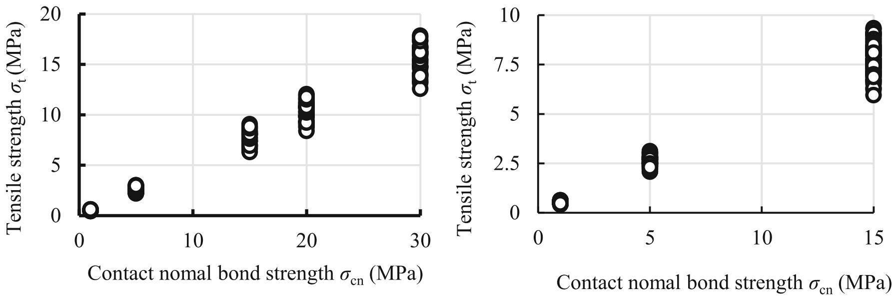
Table 2. Normal bond strength σ_{cn} and stiffness ratio k_n/k_s of different particle size (MPa).

D_{max}/D_{min}	D_{min} (mm)						
	0.2	0.3	0.4	0.6	0.8	1.0	2.0
1.2	A	A	A	A	A	A	A
1.67	A/B	A/B	A/B	A/B	A/B	A/B	/
2	A/B	A/B	A/B	A/B	A/B	A/B	/
3	A/B	A/B	A/B	A/B	A/B	/	/
4	A/B	A/B	A/B	A/B	/	/	/
5	A	A	A	/	/	/	/
6	A	A	A	/	/	/	/
7	A	A	/	/	/	/	/

3.2 Simulation Results

The simulation results of A-labeled numerical specimens are shown in Fig. 3a, the range of σ_t is 0.44–17.83 MPa. To further analyze the relation between σ_{cn} and σ_t, the macro and micro tensile strengths of numerical specimens with varying micro geometrical characteristics are linearly fitted (through the origin), where the correlation coefficients R^2 are all greater than 0.999. The slope of the linear fitting is the scale coefficient K which is 0.4199–0.6023.

The simulation results of B-labeled numerical specimens are shown in Fig. 3b, the range of σ_t is 0.40–9.33 MPa The scale coefficient K of B-labeled numerical specimens



a. σ_{cn} of A-labeled specimens b. σ_{cn} of B-labeled specimens

Fig. 3. Macro tensile strength σ_{cn} of A-labeled and B-labeled numerical specimens

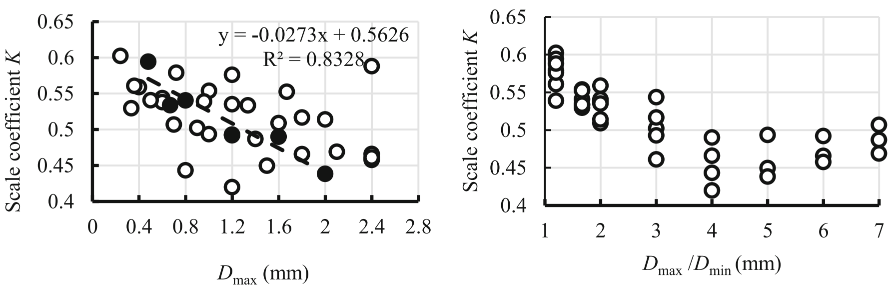
with varying micro geometrical characteristics and stiffness ratio is 0.3984–0.6223, and the correlation coefficients R^2 are all greater than 0.999.

The fitting results (correlation coefficients R^2) indicate the significant linear correlation between the micro tensile strength σ_{cn} and the macro tensile strength σ_t, which is consistent with Formula (6). Thus, K can be determined through three numerical tests with different micro tensile strengths when the other micro parameters are constant.

4 Discussion

4.1 Effects of Particle Size on Macro Tensile Strength

The effects of particle size on K is observed based on the simulation results of group A. The relation between D_{max} (D_{max}/D_{min}) and K is presented in Fig. 4a (Fig. 4b).



a. Scatter diagram of K with different D_{max} b. Scatter diagram of K with different D_{max}/D_{min}

Fig. 4. Scatter diagram of the scale coefficient K

According to Fig. 4a, with the increase of D_{max}, K shows a decreasing trend. When particle size changes, the influence of micro geometrical characteristics on K is random, which results in scattering of partial data points. The data points (k_n/k_s = 3.5, D_{max}/D_{min} = 2) with solid marks are linear fitting, $K = 0.5626 - 0.0273 \times D_{max}$, with a correlation coefficient R^2 of 0.8328. It indicates that the variation rule of K with D_{max} is consistent with that in Formula (7). However, in the application of Formula (7), the constant term and coefficient in the formula need to be modified.

In Fig. 4b, when D_{max}/D_{min} is 1–4, the influence of D_{max}/D_{min} on K is obvious and when D_{max}/D_{min} is greater than 4, it is weakened. From the aspect of theoretical model, this trend is consistent with the effect of particle diameter ratio correction term $1/(1 + d_{max}/d_{min})$ on K. From the aspect of numerical specimen, the particle diameter ratio is too large to form enough contacts, which means small particles cannot fully contact with the surrounding particles (the coordination number is about 4). Consequently, the influence of D_{max}/D_{min} on simulation results is obviously reduced.

4.2 Effects of Normal to Shear Stiffness Ratio on Macro-tensile Strength

The effects of k_n/k_s on K are observed based on the simulation results of group B, with k_n/k_s as the horizontal axis and K as the vertical axis, as shown in Fig. 5.

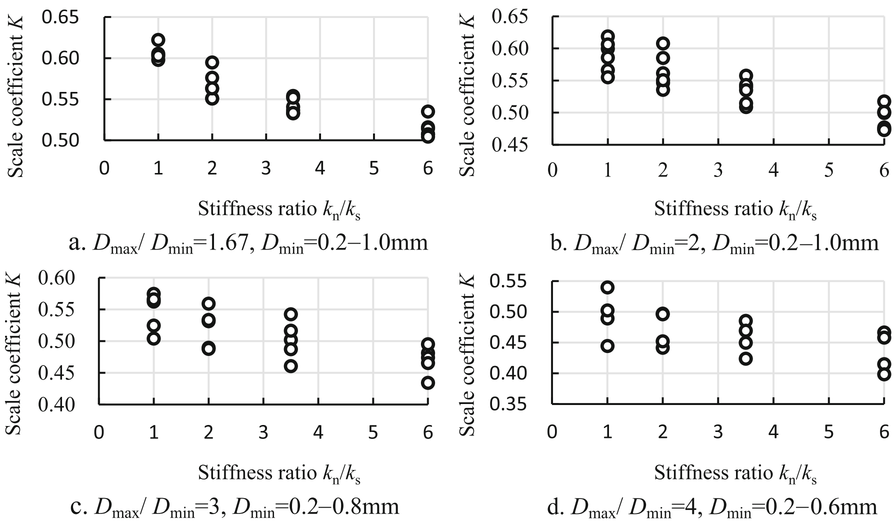


Fig. 5. Scatter diagram of the scale coefficient K with different k_n/k_s

As shown in Fig. 5, K decreases gradually with the increasing of k_n/k_s. According to Formula (7), the theoretical relation between K and k_s/k_n can be simplified as shown in Formula (10). It is clear that k_s/k_n and K exhibit a linear correlation, when micro geometric characteristics is fixed. And θ can be expressed by Formula (11), it means θ of a numerical specimen with fixed micro geometric characteristics is a constant.

$$K = a + b/(k_n/k_s) = a + b \times (k_n/k_s) \quad (10)$$

$$\theta = \arccos(\sqrt{b/2a}) \quad (11)$$

The correlation coefficient R^2 of linear fitting between K and k_s/k_n is 0.81–0.99, indicating that the statistical relationship between K and k_s/k_n is consistent with the theoretical derivation. The geometrical characteristic angle θ is 59.3°–85.4° calculated by Formula (11), which basically conforms to the relation between D_{max}/D_{min} and θ in Formula (9).

4.3 The Correction of Theoretical Formula

When the particle size (D_{max}/D_{min}, D_{max},) of numerical specimens is used directly in Formula (7), the geometrical characteristic angle θ is calculated to be 14°–46°, which is inconsistent with Formula (9), indicating that θ calculated by this method is unreasonable and the correction of geometrical parameters D_{min}/D_{max} and D_{max} is necessary. Let

$$A = \frac{K}{2(\tan\theta + \frac{\sin 2\theta}{k_n/k_s})} = \frac{1}{1 + \frac{d_{max}}{d_{min}}}(1 - \frac{d_{max}}{L}) = \frac{a}{1 + b(\frac{D_{max}}{D_{min}})}(1 - c\frac{D_{max}}{L}) \quad (12)$$

$$\sigma_t = \sigma_{cn}\frac{0.504}{1 + 0.382D_{max}/D_{min}}(1 - \frac{12.31D_{max}}{L})(\tan\theta + \frac{\sin 2\theta}{k_n/k_s}) \quad (13)$$

The value of A is calculated based on the above fitting results (K, θ) and k_n/k_s. Fitting with MATLAB software yields $a = 0.252$, $b = 0.382$, $c = 12.31$, with a correlation coefficient R^2 of 0.8952. To sum up, the theoretical relationship between macro tensile strength and micro parameters is expressed in Formula (13) within the research scope of this paper.

5 Quantitative Determining Approach of Micro Tensile Strength

According to the results of theoretical analysis and statistical analysis, the micro tensile strength of 50 mm * 100 mm specimen can be determined by the following steps.

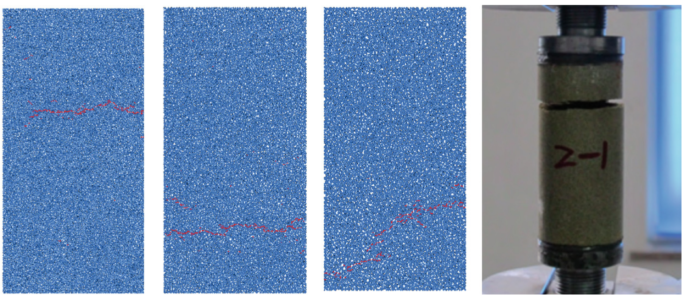
a. Preparatory work: D_{min} (D_{max}), D_{max}/D_{min} are determined according to the simulation object (rock specimen) and the arithmetic ability of computer.
b. Simulation scheme: $\sigma_{cni} = \sigma_t/K_i$ (i = 1, 2, 3) is calculated with the scale coefficient K = 0.4, 0.5, 0.6. Normal to shear stiffness ratio k_n/k_{si} is chosen adequately according to the deformation characteristics of rock specimens, such as 1, 2, 3, 4.

k_n/k_{si}	σ_{cn1}	σ_{cn2}	σ_{cn3}	K_i
k_n/k_{s1}	σ_{t11}	σ_{t12}	σ_{t13}	K_1
k_n/k_{s2}	σ_{t21}	σ_{t22}	σ_{t23}	K_2
k_n/k_{s3}	σ_{t31}	σ_{t32}	σ_{t33}	K_3
k_n/k_{s4}	σ_{t41}	σ_{t42}	σ_{t43}	K_4

c. Simulation result analysis: according to the table above, twelve direct tensile numerical tests are carried out, and the macro and micro tensile strengths are linearly fitted to obtain K_i (i = 1, 2, 3, 4). Linear fitting is performed on K_i, k_s/k_{ni} to derive the quantitative relation between K and k_n/k_s, $K = a + b/(k_n/k_s)$. When k_n/k_s is fixed, a accurate scale coefficient K can be obtained through three numerical tests.
d. Calculation of micro tensile strength: As a stiffness parameter, k_n/k_s should be obtained through simulation compression test. The micro tensile strength σ_{cn} is calculated by $\sigma_{cn} = \sigma_t/(a + b(k_n/k_s))$.

6 Verification of Solutions

A self-designed testing machine are applied to the direct tensile test to obtain tensile strength of rock by Zhang et al. [15]. According to the experimental results [15], a sandstone sample was selected as the simulation objects of verification and the tensile strength of rock sample is 2.46 MPa. Three numerical specimen with different micro parameters are established. According to the method mentioned above, the relative errors of numerical tests are 0.01%, 0.08%, 0.4%. The failure modes of numerical specimens are shown in Fig. 6, where the failure modes of No. 1 and No. 2 specimens are similar to the rock specimens. As can be seen from the figure, the failure modes of numerical specimens exhibit distinct difference due to the difference of particle diameter and the randomness of particle distribution.



(a) NO.1 (b) NO.2 (c) NO.3 (d) Rock sample[15]

Fig. 6. The failure form of three numerical models and rock sample [15]

7 Conclusion

In this paper, the simplified theoretical model was theoretically analyzed, and the statistical analysis was carried out by numerical simulation. The following conclusions can be drawn:

(1) The macro tensile strength is linear to the micro tensile, the scale coefficient K is related to the particle diameter ratio $D_{\max}/D_{\min}$, the maximum particle diameter $D_{\max}$, the normal to shear stiffness ratio k_n/k_s and the geometric characteristic angle θ.
(2) The geometric characteristic angle θ of a numerical specimen with fixed micro geometric characteristics is a constant.
(3) The theoretical formula between macro tensile strength and micro parameters is corrected.

$$\sigma_t = \sigma_{cn} \frac{0.504}{1 + 0.382 D_{\max}/D_{\min}} \left(1 - \frac{12.31 D_{\max}}{L}\right)\left(\tan\theta + \frac{\sin 2\theta}{k_n/k_s}\right)$$

(4) This paper presented a approach for determining the micro tensile strength based on direct tensile tests.

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