Numerical Simulation Method Study of Rock Fracture Based on Strain Energy Density Theory

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Abstract. Many numerical methods are carried out to study the nonlinear failure behaviors of the rock; however, the numerical simulation methods for the failed rock are still in the research stage. This paper establishes the damage constitutive equation by combining the bilinear strain softening constitutive model with energy dissipation principles, as well as the energy failure criterion of mesoscopic elements based on the strain energy density theory. When the strain energy stored by an element exceeds a fixed value, the element enters the damage state and the damage degree increases with increasing energy dissipation. Simultaneously, the material properties of the damaged element change until it becomes an element with certain residual strength. As the load increases, the damage degree of an element increases. When the strain energy stored by an element exceeds the established value of the energy criterion, the element is defined to be failed. As the number of failed elements constantly increases, failed elements interconnect and form macrocracks. The rock fracture calculation program on the basis of the preceding algorithm is successfully applied to the fracture simulation process in Brazilian splitting and intermediate crack tensile tests. This method completes the nonlinear calculation process with linear calculation, avoids singularity of numerical calculation in element fracture, and simulates the rock post-peak fracture behaviors. The simulation results agree well with the test results, indicating the accuracy and feasibility of this method for simulating the rock fracture process.

1. Introduction
As a product of geological movements, the rock is a heterogeneous material with complex mechanical properties. The rock medium usually shows strong nonlinear characteristics [1] in the deformation process. Physical and mechanical properties will be irreversible during the failure process, and this irreversible process will cause various forms of energy dissipation. According to the law of thermodynamics, energy conversion is the essential feature during the material physical process, and material failure is a kind of instability driven by energy. Therefore, studying the energy change rules and establishing the relation between energy changes and strength as well as structural failure during the rock failure process will be more conducive to reflecting strength changes and essential characteristics [2] of structural failure of the rock under the action of external load.

Since Huber firstly introduced the potential energy concept to define material damage, many scholars at home and abroad have described rock deformation behaviors through energy analysis and achieved tremendous progress [3-8]. Most work focused on tests and theoretical research and macroscopic failure behaviors of the rock were obtained through energy analysis. According to their
studies, material failures are mainly caused by irreversible internal energy dissipation; meanwhile, the energy criterion is generally significant for determining the rock failure.

The rock fracture is an entire process from damage, material progressive degradation, microcrack generation, expansion, and till penetration. Therefore, studying rock fracture from the micromechanics perspective, analysing the damage rules of tiny rock elements, and studying element failure through element energy dissipation and energy criterion can systematically show the entire rock fracture process. Currently, the most representative strain energy failure criterion is distortional strain energy density theory (fourth strength theory) \[9\]. This is a better strength theory for plastic materials; however, it is applicable only to plastic materials with the same tension and compression properties rather than triaxial equivalent tension. Therefore, besides the distortional strain energy, the volume deformation energy also needs to be considered \[10\]. The application of strain energy density theory \[11\] can comprehensively consider the preceding problems and take the strain energy density that is the sum of the volume deformation energy density and shape change energy density as the criterion of material failure. The advantage of this theory is that it can be well applied to complex geometry, loading conditions, and development situations of mixed cracks \[12\].

According to the preceding analysis, nonlinear failure behaviours of the rock are considered to simulate the rock partial failure and the entire process from microcrack generation, expansion, and complete fracture. In addition, the bilinear strain softening constitutive model is adopted by referring to document \[13\], and the energy criteria for the damage and failure of mesoscopic rock elements according to the strain energy density theory and energy dissipation principle. When the strain energy stored by an element exceeds a fixed value, the element enters the damage status. The damage degree of the element is determined based on the strain energy density and the material properties of the damaged element change until it becomes an element with certain residual strength. For rock elements entering the damage state, the energy failure criterion of strain energy density is used to determine whether the element is damaged. As the load increases, the number of failed elements gradually grows, and the failed elements interconnect and form macrocracks, causing the structural failure of the rock specimen. During the numerical simulation process, the elastic modulus reduction of damaged elements after reaching the stress extreme value is discretized. The preceding method completes the nonlinear calculation process with linear calculation, avoids singularity of numerical calculation in element fracture, and simulates the rock post-peak fracture behaviours. In this calculation method, the rock fracture calculation program is developed with Fish language in the Flac. It is successfully applied to the fracture simulation process in Brazilian splitting and intermediate crack tensile tests, indicating the accuracy and feasibility of this method for simulating the rock fracture process.

2. Strain Energy Density Theory

The rock fracture mode is affected by many factors such as the loading type, geometry, and material properties. However, the strain energy density theory can comprehensively consider these factors. The rock is assumed to be a continuum composed of many tiny structural elements and each element contains per unit volume of the material. If the element deforms under the action of external force, strain energy will be stored inside the element. In this way, the energy stored by each element is called strain energy density \(\frac{dW}{dV}\).

2.1. Determination of the Strain Energy Density Function Considering Strain Softening

According to the strain energy density theory, the strain energy density function of each element in the isothermal condition can be expressed as:

\[
\frac{dW}{dV} = \int_0^1 \sigma_{ij} d\varepsilon_{ij}
\]

According to the preceding formula, the density of strain energy stored in an element is determined by its stress \(\sigma_{ij}\) and the deformation history of strain increment \(d\varepsilon_{ij}\). This theory determines the yield
failure of the material element based on strain energy density \((dW/dV)\) and stipulates that the element fails when all strain energy absorbed by the element is equal to the energy absorbed during fracture under uniaxial tension \((dW/dV)_c\).

According to this theory, before the rock texture shows global instability under the action of load, partial failure and crack propagation already occur and seriously affect the macroscopic failure behaviors of the rock texture. The steady propagation of microcracks inside the rock will finally cause rock macroscopic fracture.

The deformation process of each rock element is accompanied with energy dissipation that will cause material progressive damage, property deterioration, and strength loss [2]. The material mechanical damage can be described by strain softening. The bilinear strain softening constitutive model of the rock under uniaxial tension in document [13] is considered, that is, the uniaxial tension stress-strain relation of the rock is simplified, as shown in Figure 1.

Figure 1. Bilinear strain softening stress-strain curve

Under the action of external force, the rock first shows elastic deformation and does not fail immediately after reaching the stress limit point U. Instead, it enters the strain softening stage and the material starts to damage. As shown in the figure, the density \((dW/dV)\) of strain energy absorbed by the material element at point A is area OUAC surrounded by the stress-strain curve. If the element is unloaded at point A, the unloading path will be along line AB and the new loading path will be along line BAF. In the process of unloading and reloading, energy represented by area OUAB is dissipated. Therefore, the density of strain energy absorbed by the material element is composed of the following two parts:

\[
\frac{dW}{dV} = \left( \frac{dW}{dV} \right)_d + \left( \frac{dW}{dV} \right)_e
\]  

In the preceding formula, \((dW/dV)_d\) is the density of strain energy dissipated OUAB while \((dW/dV)_e\) is the density of strain energy recoverable BAC.

If point A is on line OU in the elastic stage, the unloading path will be along the loading path and the material will not damage. For the material element without damage, its critical strain energy density \((dW/dV)_c\) is equal to area OUF. However, energy dissipation occurs after the material element damages. The residual critical strain energy density after damage \((dW/dV)_e^*\) is the density of strain energy regained after the element is unloaded (that is area BAF) and can be expressed as the following:
\[
\frac{dW}{dV}^* = \left(\frac{dW}{dV}\right)_c - \left(\frac{dW}{dV}\right)_d
\]  

(3)

The preceding formula indicates that a higher density of strain energy dissipated by the material element means more serious element damage and lower density of critical strain energy that can be borne.

According to the preceding analysis, larger deformation of the material element under the action of external force means a higher density of strain energy absorbed \((dW / dV)\) and lower density of critical strain energy \((dW / dV)^*_c\). When \((dW / dV) \geq (dW / dV)^*_c\), cracks start to be generated. When \((dW / dV)\) is equal to the initial critical strain energy density \((dW / dV)_c\) (that is, area OUF) of the material element, the element is completely fractured and cannot bear any load.

The bilinear constitutive relation of the preceding rock element can be simply obtained through uniaxial tensile tests. The rock texture is usually under the action of complex external force and the internal rock elements are under the combined action of tension, compression, and shear stress. The strain energy density can be obtained based on the loading history of the rock element and it can comprehensively reflect the loading status of the element. The damage status of the rock element under complex stress conditions can be determined by comparing it with the strain energy density in different stages under uniaxial tension.

2.2. Energy Dissipation and Damage Constitutive Model

According to energy opinions, after the rock shows inelastic deformation, the inelastic deformation energy the rock can bear has been significantly reduced, that is, the rock constitutive energy has decreased. This is also an expression of rock performance deterioration caused by the changes of rock microstructure [15]. After the rock element reaches the peak point of the tensile stress, it enters the strain softening stage and shows inelastic deformation and decreased material strength. The strength decrease of the material element is defined as the elastic modulus reduction and is expressed by equivalent elastic modulus \(E^*\). As shown in Figure.2, as the energy loses, the unloading peak strength decreases from point U to points G, H, I ... and the equivalent elastic modulus is \(E^*_1, E^*_2, E^*_3, \ldots\) and \(E^*_n\) respectively.

![Figure 2. Reduction of elastic modulus after energy dissipation](image)

For the sake of calculation, the equivalent elastic modulus is discretized into 20 different values:

\[
E^*(n) = \frac{(21-n)}{20}E, \quad n=1, 2, \ldots, 20
\]  

(4)
The following can be obtained according to the constitutive relation of continuous medium damage mechanics theory [16]:

$$\sigma = E(1-D)$$  \hspace{1cm} (5)

$E$ is the elastic modulus of the rock without damage.

The damage parameter $D$ of the rock element in this model is:

$$D = \frac{E - E^+(n)}{E}$$  \hspace{1cm} (6)

$n$ refers to the damage degree of the material element.

For the discretization of the equivalent elastic modulus, a larger value of $n$ means more accurate simulation results but remarkably lower calculation efficiency. $n$ is set to 20 by taking both factors into consideration, which meets related requirements.

According to the energy dissipation principle, energy dissipation is directly related to the damage and strength loss. The dissipation quantity reflects the reduction of the initial strength [2]. According to Figure.1 and formula (2), both the strain energy density and the energy dissipation increase after the rock element reaches the stress limit point. Therefore, the strain energy density is used as the criterion to determine the rock element damage and failure.

(1) When $\frac{(dW/dV)_u}{(dW/dV)_c} = 1/2(\sigma_u \varepsilon_u)$, the material element is in the elastic stage; no damage occurs; both the equivalent elastic modulus and critical strain energy density are the initial values of the element, that is, $E^+ = E$, $(dW/dV)_{u} = (dW/dV)_{c} = 1/2(\sigma_u \varepsilon_u)$.

(2) When $\frac{(dW/dV)_u}{(dW/dV)_c} > 1/2(\sigma_u \varepsilon_u)$, the material element enters the damage stage. The discretized equivalent elastic modulus $E^+(n)$ is regarded as the elastic modulus of the material element after damage. $n$ refers to the damage degree of the material element ($0 \leq n \leq 20$) and its value is determined by the strain energy density. It also can be seen from Figure.1 that the critical strain energy density $(dW/dV)_{c}$ decreases with increasing $(dW/dV)$ after the material element enters the damage stage.

(3) When $\frac{(dW/dV)_u}{(dW/dV)_c} > 1/2(\sigma_u \varepsilon_u)$, the element fails, marking the beginning of crack generation inside the material.

(4) When $\frac{(dW/dV)_u}{(dW/dV)_c} > 1/2(\sigma_u \varepsilon_u)$, according to formula (4), the damage degree of the material element reaches the largest, that is, $n = 20$; both the equivalent elastic modulus and critical strain energy density of the element change to zero; the element is completely fractured and loses the bearing capacity. To maintain the integrity of the entire structure calculation model and element continuity, the element completely fractured will be given a very small residual modulus $E_{c}^+ = 0.05E$ instead of being dug out.

2.3. Numerical Implementation

The FLAC2D finite difference numerical software is adopted to establish the rock element damage equation based on the preceding theory and develop a rock fracture calculation program with Fish language. Model loading adopts the load control stepwise loading method. In particular, equivalent tiny loads are accumulatively added to the model in turn. After calculation is balanced, the strain energy density of each element is calculated. Then, the preceding strain energy density criterion is used to determine the element damage degree and failure. After the first loading step is performed, all elements are in the elastic stage due to the small load and the strain energy density of each element is:

$$\frac{dW}{dV} = \frac{1}{2E}[\sigma_x^2 + \sigma_y^2 + 2\tau_{xy}^2 - 2v(\sigma_x \sigma_y - \tau_{xy}^2)]$$  \hspace{1cm} (7)

After loading step $i$ is performed, the strain energy density of each element is:
\[
\left(\frac{dW}{dV}\right)_i = \left(\frac{dW}{dV}\right)_{i-1} + \Delta \left(\frac{dW}{dV}\right) = \left(\frac{dW}{dV}\right)_{i-1} + \frac{1}{2} (\sigma_s^i + \sigma_s^{i-1})(\varepsilon_s^i - \varepsilon_s^{i-1}) + \frac{1}{2} (\sigma_y^i + \sigma_y^{i-1})(\varepsilon_y^i - \varepsilon_y^{i-1}) + \frac{1}{2} (\tau_{xy}^i + \tau_{xy}^{i-1})(\gamma_{xy}^i - \gamma_{xy}^{i-1})
\]

In the formula, \(i \geq 2\), \(\sigma_s^i, \sigma_y^i, \tau_{xy}^i\) are the element stress in loading step \(i\) while \(\sigma_s^{i-1}, \sigma_y^{i-1}, \tau_{xy}^{i-1}\) are the element stress in the last loading step. Similarly, the strain has the same expression way.

When the strain energy density of an element \((dW / dV) > (dW / dV)_u = 1/2(\sigma_u e_u)\), the damage degree \(n\) is:

\[
n = \frac{1}{20} \left\{ \frac{(dW / dV) - (dW / dV)_u}{(dW / dV)_e - (dW / dV)_u} \right\} = \frac{2}{20} \frac{(dW / dV) - \sigma_u e_u}{\sigma_s e_s - \sigma_u e_u}
\]

\(n\) is set to the integer part of the calculation results on the right of the equation and ranges from 0 to 20. When \(n = 0\), the element is still in the linear elastic stage and no damage occurs; when \(n = 20\), the damage value is the maximum, indicating that the element is completely fractured and loses the bearing capacity. Meanwhile, the element elastic modulus \(E^*\) is obtained by using formula (4).

The density of strain energy dissipated by the element is:

\[
(dW / dV)_d = (dW / dV) - \frac{1}{2E^*} \left[ \sigma_s^2 + \sigma_y^2 + 2\tau_{xy}^2 - 2\nu (\sigma_s \sigma_y - \tau_{xy}^2) \right]
\]

Therefore, the critical strain energy density of the element is:

\[
(dW / dV)_e^* = (dW / dV)_e - (dW / dV)_d = \frac{1}{2} \sigma_s e_s - (dW / dV) + \frac{1}{2E^*} \left[ \sigma_s^2 + \sigma_y^2 + 2\tau_{xy}^2 - 2\nu (\sigma_s \sigma_y - \tau_{xy}^2) \right]
\]

Figure.3 shows the calculation process of the damage constitutive calculation model based on strain energy density.
3. Numerical Simulation of Rock Fracture

3.1. Brazilian Splitting Numerical Simulation
This case takes the Brazilian splitting with lateral concentrated load in document [17] as an example. Figure.4 shows the calculation model. The disk diameter is 50mm and it is divided into 7860 elements. The model material adopts the marble in document [17] with the elastic modulus $E = 66.8 \text{GPa}$.
Poisson’s ratio $v = 0.33$, density $\rho = 2620 \text{Kg/m}^3$, element tension ultimate stress $\sigma_u = 20 \text{MPa}$, strain under ultimate stress $\varepsilon_u = 1.3 \times 10^{-5}$, and strain when fracture occurs $\varepsilon_f = 1 \times 10^{-4}$. The model top and bottom are imposed with load increased by 2KN in the negative y direction and positive y direction respectively.

![Figure 4](image)

**Figure 4.** Numerical calculation model of Brazil splitting

After the first 2KN load is imposed, no damage occurs inside the disk; each element is in the linear elastic stage; Figure 5 shows the distribution of the stress inside the Brazilian disk. The results of comparison of distribution rules and theoretical results of stress distribution inside the disk in document [17] show that the simulated stress distribution rules basically agree well with the theoretical distribution.

![Simulated distribution vs Theoretical distribution](image)

**Figure 5.** Comparison between theoretical and numerical results of stress distribution in Brazil disc
As the load increases, the strain energy absorbed by each element gradually increases. The energy change process of elements in the middle of the disk top is recorded, as shown in Figure.6. The strain energy density absorbed by the element \(\left(\frac{dW}{dV}\right)\) gradually increases from zero while the critical strain energy density \(\left(\frac{dW}{dV}\right)_c\) gradually decreases from \(\left(\frac{dW}{dV}\right)_c = 1000\). When they two intersect, the element fails.

![Figure 6. Curve of element strain energy density versus load change](image)

It can be seen from Figure.6 that when calculation reaches the 7th loading step, that is, 14KN load is imposed, elements in the middle of the disk top have \(\left(\frac{dW}{dV}\right) \geq \left(\frac{dW}{dV}\right)_c\), indicating that elements at both ends of the disk start to fail. When calculation reaches the 15th loading step, that is, 30KN load is imposed, partial damage at both ends is suddenly developed into complete penetration in the middle of the specimen; meanwhile, there are partial failure areas on both ends of the disk. Figure.7 shows the failure of the specimen when it is loaded to loading step 7, 12, 14, and 15.

![Figure 7. Element failure process of Brazil splitting under different loading steps](image)
Figure 8 shows the damage status of each element when the specimen fails. The damage value $n$ is expressed by the built-in variable $e_{x5}$ of the element and ranges from 1 to 20. It can be seen from the damage cloud chart of the element that the damage value of each element at the penetration point in the middle of the disk reaches the maximum value 20, indicating that elements in the middle of the disk are completely fractured and lose the bearing capacity. Elements on both ends of the disk except a small number of elements are completely fractured, and surrounding elements also show different levels of damage.

![Figure 8. Element damage status in Brazilian disc in numerical calculation.](image)

Documents [18-20] all conducted experimental studies on Brazilian disk imposed with lateral load. The results show that both ends of the disk firstly fail due to the stress concentration caused at the loading point during the splitting process of the brittle rock. As the load continues to increase, penetration occurs in the middle of the disk and the failure pie section appears on the loading points at both ends of the disk. Figure 9 shows the sketch of splitting failure of the marble under different stepping bars in document [18]. Comparison of Figure 7 and Figure 9 shows that simulated results of numerical calculation in this paper agree well with test results in the document, indicating the feasibility of this method for simulating the rock fracture.

![Figure 9. Test results of Brazilian splitting for marble in document [18].](image)

3.2. Numerical Simulation of Tensile Test with Built-in Crack

This case takes the tensile test with built-in crack in document [21] as an example. Figure 10 shows the calculation model. The specimen size is $50 \text{mm} \times 100 \text{mm}$; the length of the built-in crack is $20 \text{mm}$; the specimen is divided into 9772 elements. The specimen material adopts the rock mortar with the elastic modulus $E = 5.17 \text{GPa}$, Poisson’s ratio $\nu = 0.192$, density $\rho = 2300 \text{Kg/m}^3$, element ultimate tensile stress $\sigma_u = 2.7 \text{MPa}$, strain under ultimate stress $\varepsilon_u = 5.8 \times 10^{-4}$, and strain when fracture occurs $\varepsilon_f = 7 \times 10^{-4}$. The model top and bottom are imposed with uniform tensile load increased by 100N respectively.
The following calculation results are obtained: under the action of tensile load, stress concentration occurs on the crack tip; elements at both ends of the crack start to fail when calculation reaches the fourth loading step, that is, 400N load. Figure 11 shows the strain energy density of the first element at the left end of the crack with changing load.

![Figure 11. Curve of element strain energy density versus load change](image)

When calculation reaches the fifth loading step, that is, 500N load, penetration occurs in the middle of the specimen in the crack direction. Figure 12 shows the failure status of the model when calculation reaches loading steps 4 and 5.

![Figure 12. Element failure process of uniaxial tensile test under different loading steps](image)
Figure 13 shows the damage status of each element when the specimen fails. It can be seen from the damage cloud chart of the element that each element surrounding the crack tip shows different levels of damage due to stress concentration and that the damage value of a series of elements from both ends of the crack to the model edge reaches 20, indicating that the specimen is completely fractured along the cross section of the crack.

![Damage Status](image1.png)

**Figure 13.** Element damage status in tensile test with built-in crack

Document [21] conducted uniaxial tensile tests on mortar materials with different prefabricated crack dips on the rigidity servo testing machine. The test results show that when the tensile stress reaches a specific value, the prefabricated crack starts to initiate and then rapidly expands, causing the structural failure of the specimen. When the crack is horizontal (that is, crack dip $\alpha = 90^\circ$), wing crack is generated at the front edge of the crack and expanded in the direction of the original crack until the specimen is fractured. Finally, the fracture trace is perpendicular to the axial tensile stress direction and the fracture surface is flat. Figure 14 shows the tensile failure of horizontal crack in document [21]. Comparison of Figure 12 and Figure 14 shows that the simulated failure process and damage status in the built-in crack tensile tests of numerical calculation in this paper basically agrees with test results, indicating the accuracy and feasibility of this method in this paper for simulating the rock fracture.

![Test Results](image2.png)

**Figure 14.** Test results of uniaxial tensile test in document [21]
4. Conclusions
This numerical simulation method of rock fracture based on strain energy density theory completes the nonlinear calculation process with linear calculation, avoids singularity of numerical calculation in element fracture, and simulates the rock post-peak fracture behaviors.

(1) The tensile bilinear strain softening constitutive model is adopted to analyse the energy and damage evolution process after the rock element reaches the stress limit point from the micromechanics perspective. In addition, the criterion is created to determine element failure based on strain energy density theory. This method can well simulate the entire process of rock damage.

(2) The strain energy density of the rock element is obtained by accumulating the energy absorbed by the element after the load is imposed each time. Meanwhile, the modulus reduction of the damaged element is discretized to complete nonlinear calculation with linear calculation. A very small residual modulus is given to elements (regarded to be completely fractured) with the maximum damage values. Continuous calculation is used to implement discontinuous fracture behaviours of the rock to avoid singularity of numerical calculation in element fracture.

(3) Numerical simulation of Brazilian splitting and built-in crack tensile tests shows that the preceding method can well simulate the entire process from partial failure to structural fracture of the rock and obtain the damage evolution process of each element during the failure process.

(4) Studying rock fracture from the energy perspective can comprehensively reflect the rock strength changes and essential characteristics of the structural failure. This paper develops a rock damage numerical calculation program with Fish language in the FLAC. Compared with the theory and analytic method, this program can directly resolve various complex problems and therefore has a wider application prospect.

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