Thermal-mechanical-damage coupling model for thermal spallation in rock

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Abstract. In deep underground engineering, thermal spallation occurs when the brittle rock is suffering from high temperature. This phenomenon severely jeopardizes safety of worker and weakens the underground structure. Based on the rock thermal-mechanical-damage coupling model and theory, a novel model is proposed to explore the rock thermal spallation mechanism, including influential factors and damage evolution. The model mainly focuses on how the rock heterogeneity and micropore distribution influence thermal spallation under rapid heating. We analyse the internal temperature field, stress field, and damage field in the varying cases. This simulation results show that heterogeneity plays a pivot role in determining thermal spallation and damage in rocks. The greater the heterogeneity (more materials with larger thermal conductivity or elastic modulus), the more likely thermal spallation occurs. Moreover, the damage behaviour is also strongly influenced by micropore distribution inside the rock. The initial micropore distribution shapes preliminary damage in the rock. With the micropores increasing, the thermal spallation damage area is mostly concentrated around the micropores, as a result of the thermal stress and the existing damage together. In addition, this study indicates that the thermal damage in the rock is mainly caused by tensile stress induced by thermal expansion. The numerical results capture main features of the thermal spallation process in brittle rock, showing good agreement with the experimental observations.

1. Introduction

Shallow fossil energy is gradually exhausted, and the environmental problems are becoming increasingly serious. Therefore, to meet the development needs of human society, the exploitation of deep strata mineral resources is an effective way to solve the problem of resource shortage[1,2]. At the same time, Using an enhanced geothermal system (EGS) to extract deep thermal energy from the geothermal reservoir, the carbon emission is almost zero, which is excellent environment-friendly energy[3]. Therefore, the exploitation of deep mineral resources and EGS becomes the future development trend to solve the energy problem.

In deep rock strata, high temperatures will cause potential safety hazards to underground structures, such as a fire in tunnels and mines, which can easily lead to the failure and instability of deep rock. The specific performance is as follows: in a high-temperature environment, because of the inherent...
heterogeneity of rock and the difference of expansion characteristics of internal mineral particles\cite{4}, it is easy to produce temperature stress between particles, this leads to thermal cracking. In addition, because of the low thermal conductivity of rock, a short and rapid temperature rise will produce a large gradient of temperature gradient and expansion stress on the surface, resulting in stress concentration at the congenital crack of the rock. The temperature will cause the crack to gradually expand along the direction of stress concentration. When the stress develops to a certain extent, the crack will expand to the rock surface, causing rock damage, the process of debris falling off from the rock surface is called thermal spalling\cite{5,6}, which is the most common phenomenon in brittle rocks. Walsh\cite{6-8} proposed a numerical simulation model to study thermal spallation. In the model, the mechanical behaviours of solids and fluids are numerically simulated by the Eulerian–Godunov scheme. Meanwhile, the fracture between particles is allowed in the particles, which can well study the thermal spallation on the grain scale. Based on the basic mechanical test of Australian granite, combined with acoustic emission and electron microscopy scanning (SEM), Shao\cite{9} obtained the mechanical parameters of granite at room temperature and high temperature and analysed the thermal damage. Finally, the finite element modelling model of granite is built in ABAQUS. Saksala\cite{10} proposed a numerical model using an embedded discontinuous finite element to study the effect of pore fluid on thermal spalling of granite and discussed the three kinds of fracture scale of heterogeneous rocks under strong thermal load. Based on the concepts of linear fracture mechanics and stress intensity, Wilkinson and Kant\cite{11,12} put forward a new modelling method for rock thermal spalling, which can be used to evaluate the conditions of rock thermal cracking. Song\cite{13} et al. designed a test device to simulate thermal fracture drilling and carried out experimental verification. In this paper, a numerical model based on thermal-mechanical damage coupling was developed to explore the influence of rock heterogeneity (such as thermal conductivity and elastic modulus) and micropore distribution on the thermal spallation of rock under rapid heating condition, the influence of rock heterogeneity, initial fracture distribution and shape on rock thermal spallation is revealed. At the same time, the damage behaviour of rock is also discussed in the model.

2. Model

When the rock is exposed to a high-temperature environment, the thermal stress caused by temperature-induced rock strain changes will affect its properties, and the inevitable thermal damage will occur in the rock\cite{14}. The rock damage is the real-time characterization of each element subjected to the thermal stress, therefore, a numerical model including rock damage is the key to describe the coupled thermomechanical damage interaction. In this paper, a numerical model of directly applying temperature boundary conditions on the surface of rock samples is proposed and simulated. In the thermodynamic calculation between solids, only heat conduction is studied, and thermal convection and thermal radiation are not considered.

2.1 Thermomechanical govern modelling

The general formula for the heat conduction of rocks is given by:

\[ \lambda \nabla^2 T + Q = \rho C \frac{\partial T}{\partial t} \]  

(1)

where \( \lambda \) is the thermal conductivity of rock, \( Q \) is the heat source, \( \rho \) is the equivalent density, \( C \) is the specific heat capacity, and \( t \) is the time.

For solid mechanics, the mechanical equilibrium of the solid phase is defined as:

\[ \sigma_{y,j} - f_i = 0 \]  

(2)

where \( \sigma_{y,j} \) represents the divergence of the transpose of the Cauchy stress tensor and \( f_i \) is the body force per unit volume.
The constitutive equation of rock mechanics including volume stress component, strain component and temperature change is given by\textsuperscript{15}:

\[
\sigma_{ij} = 2G\varepsilon_{ij} + \frac{2Gv}{1-2v}\varepsilon_{ij}\delta_{ij} - \frac{2G(1+v)}{1-2v}\alpha T\delta_{ij}
\]

(3)

where \( G \) is the equivalent shear modulus of the rock, \( v \) is Poisson’s ratio, \( \delta_{ij} \) is the Kronecker delta, \( \alpha T \) is coefficient of thermal expansion (°C\(^-1\)), and the linearized strains are defined as the symmetric part of the displacement gradient \( u_{ij} \):

\[
\varepsilon_{ij} = \frac{1}{2}(u_{ij} + u_{ji})
\]

(4)

According to the above formula, thermal mechanical coupling governing equation, also the governing equation of rock deformation under the influence of temperature change can be obtained as follows:

\[
Gu_{i,kk} + \frac{G}{1-2v}u_{k,ki} - \frac{2G(1+v)}{1-2v}\alpha T\delta_{ij} + f_i = 0
\]

(5)

\[2.2 \text{ Damage model of rock heterogeneity}\]

In order to express the heterogeneity of rock, mechanical parameters of rock, such as strength, Young's modulus, and Poisson's ratio, are defined according to Weibull distribution\textsuperscript{16-21}:

\[
f(u) = \frac{m}{u_0} \left( \frac{u}{u_0} \right)^{m-1} e^{- \left( \frac{u}{u_0} \right)^m}
\]

(6)

where \( u \) refers to the mechanical parameters of rock (such as strength, elastic modulus, Poisson's ratio, etc.). The definition of \( u_0 \) is related to the average value of mechanical parameters. \( m \) is the shape function of the Weibull distribution function, also known as the degree of rock heterogeneity. A higher value of \( m \) will represent a more uniform rock.

When the stress condition of rock meets the maximum tensile stress criterion or Mohr-Coulomb criterion, the rock damage begins to occur. The damage threshold functions \( F_1 \) and \( F_2 \) are defined as follows:

\[
F_1 = -\sigma_3 - f_t = 0
\]

\[
F_2 = \sigma_1 - \sigma_3 \frac{1 + \sin \theta}{1 - \sin \theta} - f_c = 0
\]

(7)

where \( f_t \) and \( f_c \) are uniaxial tensile and compressive strength (Pa), respectively, \( \sigma_1 \) and \( \sigma_3 \) are first and third principal stresses (Pa), respectively, \( \theta \) is the internal frictional angle (°), the elastic modulus of the damaged rock is expressed as:

\[
E = (1 - D)E_0
\]

(8)

where \( D \) represents the damage variable, \( E \) and \( E_0 \) are the Young's modulus (Pa) of the damaged and the undamaged element. Under any stress and initial conditions, the tensile stress criterion is applied preferentially. In other words, the maximum tensile stress criterion is first applied to judge
whether the elements are first damaged in tension or not. Only elements that survive this test will be checked for damage in shear using the Mohr–Coulomb criterion.

In terms of the damage constitutive law shown in Fig. 1, the damage variable for the rock can be calculated as[18]:

\[
D = \begin{cases} 
0 & F_1 < 0 \text{ and } F_2 < 0 \\
1 - \left( \frac{\varepsilon_1}{\varepsilon_3} \right)^n & F_1 = 0 \text{ and } dF_1 > 0 \\
1 - \left( \frac{\varepsilon_1}{\varepsilon_3} \right)^n & F_2 = 0 \text{ and } dF_2 > 0 
\end{cases} 
\]

(9)

where \( \varepsilon_1 \) and \( \varepsilon_3 \) are the major and minor principal strains. \( \varepsilon_{i0} \) and \( \varepsilon_{c0} \) are the maximum tensile and maximum compressive principal strains when tensile and shear damage occurs, respectively, and \( n \) is a constitutive coefficient specified as 2. When \( F_1 < 0 \) and \( F_2 < 0 \) the applied stress is insufficient to satisfy the maximum tensile stress criterion and the Mohr–Coulomb failure criterion, respectively. \( F_1 = 0 \) and \( dF_1 > 0 \) implies rock damage in the tensile mode when the stress state satisfies the maximum tensile stress criterion and the rock is still under load. \( F_2 = 0 \) and \( dF_2 > 0 \) implies rock damage in the shear mode when the stress state satisfies the Mohr–Coulomb failure criterion and the rock remains loaded.

Aiming at the practical problem of thermal spalling, a novel numerical model was implemented into MATLAB with COMSOL which including the thermal-mechanical damage coupling constitutive model to explore the corresponding relationship between different thermal environments and rock damage. The numerical model and experimental equipment of thermal spalling are shown in Fig.2 and Fig.3 respectively.
The numerical definition of granite in the model is shown in Table 1.

Table 1 Thermo-physico-mechanical parameters of the numerical model

| Symbol                                    | Value       | Unit |
|-------------------------------------------|-------------|------|
| Homogeneity index                         | 5           | –    |
| Mean Young’s modulus                      | 43          | GPa  |
| Mean UCS                                  | 350         | MPa  |
| Poisson ratio                             | 0.25        | –    |
| Ratio of compressive to tensile strength  | 10          | –    |
| Friction angle                            | 30          | °    |
| Specific heat capacity                    | 900         | J/kg K |
| Coefficient of linear thermal expansion   | $4.6 \times 10^{-6}$ | 1/K  |
| Thermal conductivity                      | 3.48        | W/m K |

Thermal spalling refers to the phenomenon that brittle rock is suddenly exposed to high temperature, which is affected by the internal thermal stress of rock, resulting in fracture and rock failure. Therefore, to simulate the real mechanical response of rock in this environment, the model is heated by the upper heat source continuously, and the initial heating temperature is set to 80°C with the increase heating rate of 3°C/min.

2.3 Influence of heterogeneity on thermal spalling of granite

Because of the different mechanical parameters of each element, heterogeneous material will cause unequal thermal expansion of each element under the influence of temperature gradient, which will lead to non-uniform distribution of stress state in the rock. It is highly probable to produce local stress...
concentration and cause partial damage to the rock. The damage crack caused by local stress concentration will produce more large-scale stress concentration distribution, which will conduce thermal spallation. Walsh\(^5\) pointed out that the larger the heterogeneous, such as surface roughness, grain size, and thermal conductivity distribution, the more conducive to thermal spalling. Weibull distribution is introduced to describe the relationship between heterogeneity and thermal spalling of different rocks. The probability density function of the Weibull distribution is shown in Eq\((6)\). In this paper, the heterogeneity of rock is 10 and 6 respectively, and the thermal spallation of two kinds of rocks are studied, which are named Gr-1 and Gr-2.

The thermal spallation of the two rocks is simulated based on the novel numerical model. The results show that the two kinds of rocks show an obvious thermal spalling phenomenon. With the increase of temperature, the thermal stress increases until the failure criterion shown in Fig.1 is met. The element is damaged and gradually expands. In this process, the thermal damage in the model will degrade the elastic modulus and strength of each element of rock. According to the elastic modulus distribution, except for the natural cracks of the rock, there are some damaged elements located in other areas, especially the direct heating part, generally speaking, the damage is mainly concentrated at the end of natural cracks, and develops to the rock surface, resulting in the obvious thermal spallation. The damage of Gr-1 and Gr-2 at different temperatures is shown in the Fig.4. It is obvious that the heterogeneity has a great influence on the thermal spallation.

2.4 Influence of micropore distribution on thermal spalling of granite

A large number of micropores are distributed in natural rock, and the existence of micropores will weakening the strength of rock. To explore the influence of pristine micropores distribution on thermal spalling effect, some random micropores (Gr-3 case) are added on Gr-1 with the same heating path and mode.

The damage of Gr-3 at different temperatures is shown in the Fig.5 to compare with Gr-1. It is obvious that the heterogeneity has a great influence on the thermal spallation.
It is quite obvious in Gr-3 that with the increase of the number of micropores, the thermal stress and the existing damage work together, resulting in the damaged area of rock mainly concentrated around the micropores and the end of natural cracks. Compared with Gr-1, the existence of micropores reduces the threshold of thermal spallation, the temperature of initial rock structure with microcracks, crack propagation and crack developed to the rock surface of Gr-3 are all lower than those of Gr-1. Therefore, the damage behaviour is strongly affected by the distribution of micropores in the rock. The denser the pore distribution is, the greater the potential tendency of thermal spallation is.

2.5 damage behaviour of thermal spallation
The damage of rock is a dynamic behaviour that alters with the change of external stress conditions. In the thermal spallation, because of the low thermal conductivity of granite, the temperature gradient produces local stress concentration near the natural fracture. If the temperature stress in the region meets the damage criterion proposed in Eq.(9), the damage distribution in the region will be similar to that in the temperature stress distribution. With the increase of the external temperature, the higher temperature stress is caused, and the damage in granite is further expanded.

In this paper, according to the Mohr-Coulomb criterion and the maximum tensile stress criterion, the damage model can directly represent the damage of rock. When $D < 1$, it means that the rock has tensile damage and vice versa.

According to the damage results in Gr-1, Gr-2, and Gr-3, as shown in the Fig.6, it can be seen that the damage evolution of rock is completely consistent with the elastic modulus. In addition to natural cracks, it is easier to cause damage in the inner part of the sample with large heterogeneity. At the same time, the damage caused by thermal spallation is tensile damage, which is in good agreement with the actual test.

3. Conclusions
This study develops a novel thermal mechanical damage (TMD) constitutive model to evaluate the thermal spallation and damage behaviour of rock. By applying a rapid heat transfer, the thermal stress-induced failure is linked with the damage model, and the basic conditions of rock thermal fracture are
evaluated according to the model. Based on the results and the observations reported in this study, the following conclusions are drawn:

(1) External high-temperature heat source causes direct damage to the outside of the rock, while the thermal damage will also occur in the internal pores. With the continuous heating of the heat source, the damaged areas will also grow, thus changing the mechanical properties of the rock.

(2) The elastic modulus and strength of rock will keep decreasing with the increase of temperature. The numerical model results are in good agreement with the actual test.

(3) During thermal treatment, the state of the microstructure of the rock is controlled by thermal expansion. Numerical results demonstrate that thermally-induced damage is dominated by tensile damage.

(4) Heterogeneity plays a pivot role in determining thermal spallation and damage in rocks. The greater the heterogeneity (more materials with larger thermal conductivity or elastic modulus), the more likely thermal spallation occurs.

(5) The damage behaviour is also strongly influenced by micropore distribution inside the rock. The initial micropore distribution shapes preliminary damage in the rock. With the micropores increasing, the thermal spallation damage area is mostly concentrated around the micropores, as a result of the thermal stress and the existing damage together.

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