Thermally induced failure process of brittle rocks based on a thermo-mechanical coupling model

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Abstract. The thermal expansion and the extraction characteristics of a rock are observed in a common phenomenon caused by the rock’s exposure to significant temperature differences. A thermally induced rock damage is a complex process full of uncertain physical and mechanical processes. Hence, investigating the mechanism of brittle materials is significant for both scientific and engineering applications. This study proposes a thermo-mechanical coupling model based on a continuous-discontinuous element method to simulate the thermal cracking processes in brittle rocks. In this micro-mechanical model, the rock matrix is simulated as an assembly of blocks bonded to each other. A spring model is employed to model the contacts in the blocks to simulate the mechanical deformation properties, while a thermal model is applied between their bonds to simulate heat conduction. The model validity is verified herein. Furthermore, the cracking process of brittle materials under the thermal stresses caused by the temperature gradient is studied using a thick-wall cylinder model. Consequently, the simulation results show that the microscopic crack initiation and propagation processes can be reasonably simulated at the cooling stage using the thermo-mechanical coupling model. Different geological and operation conditions are also further studied to reveal their effects on the patterns of induced fractures. This study provides a possible method for analyzing the thermal damage process and mechanism of brittle materials.

1. Introduction

A rock is composed of different mineral grains, and rock damage usually occurs when a rock block experiences a high thermal gradient [1]. The thermal stress caused by differences in the thermal conductivity of mineral grains is produced, even in uniform heating or cooling conditions [2]. Investigating the thermally induced rock damage is greatly important in underground rock engineering, especially in the fields of geothermal and oil exploitation, nuclear waste storage, and some deep metal mines. Hot dry rock exploitation is a typical engineering practice, in which thermal cracking is utilized to form a fracture network for enhancing the permeability of a geothermal reservoir. Therefore, rock thermal fracturing has great application prospect in the development of the geothermal energy extraction technology. Thermal cracking and its temperature effect on the mechanical properties of rocks have been extensively studied through different research methods [3–6]. A large amount of research involving theoretical deduction, laboratory experiment, in-situ testing, and numerical simulation has been performed in an attempt to understand the thermally induced rock damage. The majority of these studies investigated the thermally induced damage at the sample scale. In addition, rocks or models were considered to be continuous or discontinuous with pre-existing fractures [1–6]. Although
previous studies solved many cognitive and technical problems, many intractable problems are still caused by the algorithms of numerical methods and models. Rock thermal fracturing is affected not only by the rock character and structure, but also by the heating mode and velocity. This study proposes a thermo-mechanical coupling model based on a continuous–discontinuous element method to study the rock thermal fracturing mechanism. The fracture initiation and propagation characteristics induced by rock specimen cooling are studied. Furthermore, the thermal cracking mechanism is discussed and compared with the experimental results and other numerical results.

2. Modeling methodology

2.1. Continuous–discontinuous element method

The continuous–discontinuous element method (CDEM) is a dynamic explicit algorithm based on the element fracture under a Lagrange system [7]. This algorithmic method takes the advantages of the continuous model and the discrete element method and is based on a time-dependent explicit iteration using dynamic relaxation. The block deformation is calculated with a finite element method, while the interfaces between the blocks are calculated with a bond or contact spring model. The progressive failure process of rocks from continuous deformation, crack growth, to failure can be simulated with this numerical method [8–11]. Figure 1 presents the basic concepts and model.

![Figure 1. Basic concept and models: (a) geometrical and (b) interface models](image)

The governing equation of the CDEM is established with the Lagrange equation. The kinetic equilibrium equation can be obtained as follows from the Lagrange equation:

$$\sigma_{ij} + f_i - \rho \ddot{u}_i - \mu \dot{u}_i = 0$$  \hspace{1cm} (1)

where, $\sigma_{ij}$ is the stress tensor; $f_i$ is the body force; $\rho$ is the density; $\dot{u}_i$ represents the velocity vector; $\ddot{u}_i$ denotes the acceleration vector; and $\mu$ is the damping coefficient.

The equilibrium equation of momentum in Eq. (9) can be transformed into the following matrix form in an element using the variation formulation:

$$M\ddot{u}(t) + C\dot{u}(t) + Ku(t) = F(t)$$  \hspace{1cm} (2)

where, $M$, $C$, and $K$ represent the mass, damping, and stiffness matrices, respectively; $\ddot{u}(t)$, $\dot{u}(t)$, and $u(t)$ denote the vectors containing the nodal accelerations, displacements, and velocities at time point $t$, respectively; and $F(t)$ is the external loading force expressed as follows:

$$F(t) = F_b + F_p + F_s + F_t$$  \hspace{1cm} (3)
where, \( F \) is the body force; \( F_p \) is the fluid pressure on the fracture surface; \( F_s \) is the spring force; and \( F_t \) is the force on the traction boundary. The strain–displacement relationship is given as follows:

\[
\varepsilon = \frac{1}{2} \left( u_{i,j} + u_{j,i} \right) 
\]

(4)

The constitutive relation law is given as follows:

\[
\sigma_{ij} = C_{ijkl} \varepsilon_{kl}
\]

(5)

The boundary conditions are given as follows:

\[
u_i = \bar{u}_i, \quad \sigma_{ij} n_j = \bar{\sigma}_i
\]

(6)

The initial conditions are given as follows:

\[
u_i(x, y, z, 0) = \bar{u}_i^0(x, y, z) \]

\[
\sigma_{ij}(x, y, z, 0) = \bar{\sigma}_{ij}^0(x, y, z)
\]

(7)

In Eqs. (4)–(7), \( \varepsilon \) and \( \varepsilon_{ij} \) represent the strain tensor versus coordinate; \( \sigma_{ij} \) is the stress tensor, \( \sigma_{i,j} \) and \( \sigma_{j,i} \) are both the first-order partial derivatives of displacement versus coordinate; \( C_{ijkl} \) is the stress–strain tensor; \( \bar{u}_i \) is the displacement on the displacement boundary; \( \bar{u}_i^0 \) is the displacement on the initial displacement boundary; \( \bar{\sigma}_i \) is the confining stress on the external force boundary; and \( \bar{\sigma}_{ij}^0 \) is the confining stress on the initial external force boundary.

2.2. Thermo-mechanical coupling model description

The CDME blocks are composed of one or more finite elements, and the interfaces between the blocks are springs. The discontinuous deformation between the blocks is mainly realized by spring deformation and fracture. Therefore, from the model structure perspective, the heat conduction in the CDEM model includes the heat conduction inside the blocks and that on the contact boundary (i.e., Interface, Figure 1).

The heat conduction inside the block is described by the classical heat conduction model used in a continuous medium. The finite volume method is used to solve the heat conduction process inside the block. Each block is composed of several cells; thus, the cell heat flow rate is calculated according to the node temperature. The heat flow through each node is then calculated according to the cell heat flow rate. In the presence of multiple units, the flow rate at the common node must be superimposed, and the total heat flow rate of the node can be obtained by adding up the external heating and contact boundary heat flow rates. The temperature change amount is then calculated according to the total heat flow. Finally, the temperature of the next calculation step can be obtained according to the temperature of the current step.

2.2.1. Heat conduction inside the block

The finite volume method is used to solve the heat conduction process inside the block. Each block consists of several units; thus, the unit heat flow rate based on the node temperature \( q_i \) is given as follows:

\[
q_i = -\frac{k}{V} \sum_{j=1}^{n} T n_j \Delta S^j
\]

(8)
where, \( N \) is the number of faces contained in a certain unit (\( N = 3 \) in the triangular unit; \( N = 4 \) in the tetrahedral unit); \( \Delta S^j \) is the \( j \) face area; \( \vec{n}_i^j \) is the component of the normal vector outside the unit of the \( j \) face in the \( i \) direction; and \( \overline{T} \) is the average value of the temperature on the \( j \)th surface. 

The heat flux \( q \) flow through each node is obtained as follows according to the unit heat flow rate:

\[
q = \sum_{j=1}^{M} q_j \vec{n}_i^j \Delta S^j \quad \frac{M}{M}
\]

where, \( M \) represents the number of faces associated with a node in a cell (\( M = 2 \) for a triangle; \( M = 3 \) for a tetrahedron), and \( j \) is the face number.

In the presence of multiple units, the flow at the common node must be superimposed and added to the external heating flow and the contact boundary heat flow to obtain the total heat flow \( Q_t \) of the node.

\[
Q_t = \sum_{j=1}^{N_c} q + Q_{app} + Q_{cn}
\]

where, \( N_c \) is the number of cells related to a node; \( Q_{app} \) is the external heat flow boundary; and \( Q_{cn} \) is the heat flow obtained at the contact boundary.

The temperature change \( \Delta T \) is calculated as follows according to the total heat flow \( Q_t \):

\[
\Delta T = \frac{Q_t \Delta t}{C \rho V_{node}}
\]

where, \( \Delta t \) is the time step, and \( V_{node} \) is the node volume.

The temperature of the next calculation step is calculated as follows according to the temperature of the current time step:

\[
T(t + \Delta t) = T(t) + \Delta T
\]

2.2.2. Heat conduction on the contact boundary

The heat conduction on the contact boundary is described by a one-dimensional (1D) heat conduction model. Furthermore, the penalty function method is used to solve the heat conduction process. A half-spring–half-prism coupling model is used to describe and mark the contact pairs to quickly establish a complex contact relationship in a discontinuous medium system. For brevity, only the 1D heat conduction equation on the contact interface is given.
Figure 2. Two types of heat conduction models on the contact interface: (a) point-to-surface contact type and (b) edge contact type

The 1D heat conduction equation on the contact interface is given as follows:

\[ Q_c = -k \frac{T_1 - T_2}{\Delta L} A \beta \]  

(13)

where, \( \Delta L \) is the characteristic thickness of the contact boundary; \( A \) is the characteristic area of the half-spring or half-edge; and \( \beta \) is the stiffness factor representing the resistance of the contact interface to heat transfer. The larger the stiffness factor, the smaller the resistance.

2.3. Model geometry

The aforementioned calculation method was applied to simulate the process of the thermal cracking phenomenon. Accordingly, a thick-walled cylinder with an inner diameter \( r = 0.04 \) m and an outer diameter \( R = 0.5 \) m was established for the subsequent simulation. Figure 3 shows the basic geometry and setup. The model represents a two-dimensional horizontal section of a geothermal reservoir. A vertical wellbore was excavated at the center of the model to serve as the heating/cooling hole during the simulation. Fixed displacement boundary conditions were set to mimic the common laboratory tests (Figure 3a), while constant stress boundary conditions were adopted to model the actual stress environment (Figure 3b). In this case, the stresses in the x (H) directions on the model boundary were 15 MPa, whereas those in the y (h) directions on the model boundary were 15 MPa and 10 MPa under different simulation conditions.

Figure 3. Numerical model setup: (a) displacement constraint conditions and (b) stress boundary constraints
2.4. Input data
This study focuses on thermally induced fracture initiation and propagation under different geological and operation conditions. Thus, the thick-walled cylinder was assumed to be a homogeneous isotropic medium for eliminating the potential influences of the heterogeneous pore and fracture structures. The rock mechanical parameters used in the couple model were calibrated through a series of trial-and-error experiments. The micro-parameters were also calibrated to match the macro properties of traditional granite, including the elastic modulus, peak strength, and Poisson’s ratio. Table 1 presents the physical and mechanical parameters of the model used herein.

| Index                  | Value   |
|------------------------|---------|
| Elastic modulus/Pa      | 5e10    |
| Poisson’s ratio         | 0.25    |
| Density/m³/kg           | 2500    |
| Tensile strength/Pa     | 8e6     |
| Cohesive strength/Pa    | 3e6     |
| Friction angle/°        | 40      |
| Dilation angle/°        | 15      |
| Thermal conductivity    | 3.49    |
| Specific heat capacity  | 3e−5    |
| Thermal expansion coefficient | 1      |

3. Results and discussion
The numerical mimic laboratory thermal experiments of heat conduction, thermal deformation, and thermal damage under different thermal gradients and boundary conditions were successfully performed according to the proposed thermo-mechanical coupling method. The steady-state and transient heat conduction and the thermal deformation induced by the temperature changes were a continuous deformation and thermal coupling process because the temperature value and the thermal gradient were at a low level, where the thermally induced stress did not exceed the material strength. In contrast, unbalanced thermal cracking and fracture network will occur if significant thermal stress is induced by a high thermal gradient. The initiation of thermally induced fractures mainly depends on the non-uniform thermal stress field. From a microscopic point of view, the difference in the thermal conductivity and thermal expansion coefficient of the rock mineral particles is the essential reason for the emergence of the differential thermal stress in rocks.

3.1. Steady-state heat conduction
The thermal conductivity coefficient plays a vital role in the heat transmission process. A steady-state heat conduction model was established and simulated herein without considering the thermo-mechanical coupling process to verify the reliability of the foregoing heat conduction model in the actual calculation. An initial temperature of 0 °C was set for the whole model. Accordingly, a constant temperature of 100 °C was set at the inner wall of the cylinder to mimic the practical heating process. Figure 4 depicts the final distribution of the temperature simulated by the coupled model.
Figure 4. Distribution of the temperature simulated with steady-state heat conduction

Figure 5. Distribution of the temperature simulated with transient heat conduction

3.2. Transient heat conduction

The transient thermal transmission and dissipation properties of rocks are important research contents in the study of the rock thermal failure. A transient heat conduction simulation was performed herein to investigate specific rock thermodynamic properties and verify the correctness of the established heat conduction model.

An initial temperature of 100 °C was set for the whole model. A constant temperature of 0 °C was set at the inner wall and outer boundary of the cylinder to mimic the practical heating process. Figure 5 illustrates the final temperature distribution simulated by the coupled model. The model’s temperature gradually decreased at the inner wall and the outer boundary of the cylinder. Moreover, the decreasing temperature zone expanded from the inner wall and the outer boundary to the middle area.

3.3. Thermally induced fractures in a high thermal gradient

Temperature gradient and thermal expansion are considered as two important external and internal factors causing the tensile stress formation inside a rock, which consequently leads to its thermal fracture. Figure 6 displays the final thermally induced damage of the rock specimen obtained by the coupled model under a high thermal gradient and a continuous cooling process.
When the inner hole temperature continued to decrease, a number of radial fractures were generated from the inner hole outward because of the extraction and the compression deformation of the rock caused by the thermal gradient (Figure 6). The macroscopic failure behaviors of the numerical simulation were similar to those found in the laboratory experiment. In both cases, the fractures initiated from the rock specimen surface. The high tensile tangential stresses induced by the temperature changes were thought to be the induced causes of the thermal fractures. The damage of the rock specimens mainly depended on the strength and thermal expansion coefficients of the material. When the local tensile stress in the vicinity of the inner wall exceeds the material strength, micro-cracks will be induced, and the crack coalescence will eventually evolve into macro-cracks and thermal fractures. The inner wall cracking influences the heating conduction of the specimen. These newborn micro-cracks and fractures will not only hinder the subsequent process of heat transfer, but will also aggravate the stress field imbalance, which will consequently cause a new thermal damage.

3.4. Influences of temperature change velocity on thermally induced fractures
The stress change in the rock mass is caused by the mineral grain radii and bond force thermal change. The differential thermal expansion/extraction rates of the mineral grains and the thermally induced strain changes could exert an important effect on the mechanical response. In this perspective, the temperature change velocity will inevitably affect the pattern of the thermally induced fracture network. Therefore, we performed a comparative study on the thermal fracture of rocks caused by two different cooling rates. Figure 7 depicts the final thermal damage of the rock specimen. The comparison chart illustrated that the model with a faster cooling rate produced more cracks than that with a slower cooling rate. In terms of the crack shape and distribution, the faster the cooling rate, the higher the number of micro-cracks formed around the inner hole. Furthermore, the higher the crack roughness, the higher the number of branch cracks formed. Therefore, for some projects (e.g., enhanced geothermal systems), the rapid cooling method can be used to obtain more favorable artificial fracture networks.
3.5. Influences of stress ratios on the thermal cracking patterns

The in-situ stress ratio is a vital geological parameter in the process of a thermally induced damage. A group of simulations was performed with stress boundary conditions and high thermal gradient to investigate the effects of the stress ratios on the thermal fracture initiation and propagation. The stress ratio defined as the ratio of $\sigma_H/\sigma_h$ was studied herein to evaluate its effects on the thermal cracking response.

Figure 8 shows the simulated fracture distribution with stress ratios equal to 1.5 and 1.0. The thermally induced fractures have different orientations and patterns under different stress boundary conditions. The simulation results showed that a large stress ratio is conducive to the formation of branching fractures, which can increase the complexity of the fracture network morphology. However, no particular relationship was found between the dominant direction of the crack and the direction of the maximum principal compressive stress.

4. Conclusions
A thermally induced rock damage is a complex process full of uncertain physical and mechanical processes. This study proposed a thermo-mechanical coupling model based on a continuous–discontinuous element method to simulate the thermal cracking processes in brittle rocks. The thermal cracking caused by the temperature gradient was studied herein using a thick-wall cylinder model. The fracture initiation and propagation characteristics induced by the rock specimen cooling were studied. Furthermore, the thermal cracking mechanism was discussed and compared with the experimental results and other numerical results. Different geological and operation conditions were also studied to reveal their effects on the patterns of the thermally induced fractures.

The proposed thermo-mechanical coupling method showed that the initiation of the thermally induced fractures mainly depended on the non-uniform thermal stress field. The difference in the thermal conductivity and thermal expansion coefficient of the rock grains is the essential reason for the emergence of the differential thermal stress in rocks. The rock specimen damage mainly depended on the strength and thermal expansion coefficients of the material. The differential thermal expansion rates of the mineral grains and the thermally induced strain changes could exert an important effect on the mechanical response. When the local tensile stress exceeds the material strength, micro-cracks will be induced and will eventually evolve into macro thermal cracking. This numerical study found that the model with a faster temperature change rate could result in more branch cracks and a higher crack roughness. Moreover, a high in-situ ratio is beneficial in forming branching fractures, which can increase the complexity of the fracture network morphology.

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