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A coupled thermo-mechanical model based on the combined finite-discrete element method for simulating thermal cracking of rock

Chengzeng Yan^a, Hong Zheng^{b,*}^a Faculty of Engineering, China University of Geosciences, Wuhan 430074, Hubei, China^b State Key Laboratory of Geomechanics and Geotechnical Engineering, Institute of Rock and Soil Mechanics, Chinese Academy of Sciences, Wuhan, Hubei, China

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ABSTRACT

Based on a combined finite-discrete element method (FDEM), this study builds a coupled thermo-mechanical model (termed FDEM-TM) to simulate thermal cracking of rock. The coupled thermo-mechanical model consists of two major parts. In the first part the temperature distribution of the system is analyzed based on the heat conduction equation. In the second part the thermal stress caused by temperature change is added to perform mechanical fracture calculation. Based on these two parts, we can model rock fracture driven by thermo-mechanical coupling. Three examples with analytic solutions are used to verify the correctness of the model in dealing with the problems of steady-state heat conduction, unsteady-state conduction, and thermal-mechanic coupling, respectively. In addition, an example of thermal cracking is also given and compared with the experimental results. The simulation results are in excellent agreement with the analytical solutions or experimental results, verifying the correctness of the coupled thermo-mechanical model to simulate thermal cracking. The proposed method provides a new tool for thermal-mechanical coupling problems in geothermal exploitation.

1. Introduction

Rock is composed of different mineral grains or crystals cemented together. The thermal expansion characteristics of different mineral grains are different. Consequently, even in the case of uniform heating, thermal stress will be produced in rock. Once the stress exceeds the strength of the material, rock will generate micro-cracks. If these micro-cracks constitute fracture networks, macroscopic thermal cracking will emerge. From geothermal exploitation, nuclear waste storage, oil exploitation, coal seam gas safety drainage and crustal evolution, to earthquake mechanism research, we need to consider rock thermal cracking. For example, in a nuclear waste repository, we should prevent rock thermal cracking induced by decay heat of nuclear waste, because rock fracture will cause radionuclide migration contamination. However, in geothermal extraction and petroleum exploitation, thermal cracking can be utilized to form fracture network in rock, which will enhance the permeability of rock, thereby increasing oil production and geothermal acquisition amount. Consequently, the study of thermal cracking has important theoretical and engineering significance.

Many scholars have been studied thermal cracking and the effect of

temperature on mechanical properties of rock through experiment.^{1,2} Another mean of studying thermal cracking of rocks is numerical simulation. The main numerical methods for simulating thermal cracking can be divided into two categories: continuum-based methods and discontinuum-based methods.

For continuum-based methods, Tang et al.^{3,4} established a coupled thermo-mechanical model in RFPA to simulate thermal cracking process of brittle materials. Similarly, Li et al.^{5,6} built an initially thermo-mechanical-damage model (TMD) and a temperature-seepage-stress-damage (THMD) model to explore meso-structural damage and evolutionary mechanisms of rock under the effect of multi-physics coupling. Using Flac3D, Kwon and Cho⁷ studied the effect of excavation damage zone on rock behavior of thermo-mechanical coupling and hydraulic-mechanical coupling, but it cannot simulate thermal cracking of rock. Ngo et al.⁸ proposed a new thermal damage model based on finite element method, it is possible to model softening behavior of brittle materials under the effect of load, including temperature change. Dempsey et al.⁹ studied the stress change and permeability enhancement caused by fluid injection in geothermal systems with thermo-hydraulic-mechanical simulation program (FEHM).

* Corresponding author.

E-mail addresses: yanchengzheng86@gmail.com (C. Yan), hzheng@whrsm.ac.cn (H. Zheng).

For discontinuum-based methods, using discontinuous deformation analysis (DDA), Jiao et al.¹⁰ proposed a coupled thermo-mechanical model that can simulate the rock fracture induced by temperature stress. Wanne and Young¹¹ performed a numerical simulation of rock thermal cracking based on BPM model. Feng et al.^{12,13} proposed a novel discrete thermal element method (DTEM) for modeling heat transfer in systems comprising a large number of circular particles. Xia and Zhao^{14,15} presented a new thermo-mechanical coupled particle model to simulate rock damage caused by thermal stress. The difference between the model and the traditional thermo-mechanical particle model is that the elastic modulus and strength parameters are defined as a function of temperature explicitly. Using the particle flow code, Dedecker et al.¹⁶ studied the effect of high pressure fluid and thermal stress on rock mechanical behavior. Ali and Bradshaw^{17,18} studied the effect of microwave heating on the mineral crushing using BPM model in particle flow code. Vargas-Escobar¹⁹ proposed a particle thermal dynamics (TPD) for simulating heat transfer in particle material.

Although the above numerical methods have achieved some good results in the simulation of thermal cracking, they did not consider contacts explicitly, or limit to solve small-scale problems. To simulate continuum fracture, Munjiza et al.^{20–22} proposed a combined finite-discrete element method (FDEM), which is very suitable to simulate rock fracture. Since stress and strain in the triangular element are calculated based on finite element method, the concept of stress and strain in continuum mechanics are well preserved in FDEM. Also, in order to reflect discontinuities easily, discrete element method is used to handle contacts in FDEM. In addition, explicit algorithm is used, which enables FDEM to solve large-scale problems. Because of the obvious advantages of this method, FDEM has gained rapid development and extensive application in recent years. For example, a FDEM software package called the Hybrid Optimization Software Suite (HOSS) is developed by Rougier and Knight,^{23,24} which includes a large strain finite element formulation addressed in detail in Munjiza et al.²⁵ Lei et al.²⁶ developed a generated anisotropic deformation formulation for geomaterials. Mahabadi et al.²⁷ performed three-dimensional FDEM numerical simulation of failure processes observed in Opalinus Clay laboratory samples. Lisjak et al.²⁸ studied the failure mechanisms around unsupported circular excavations in anisotropic clay shales using FDEM. Tatone and Grasselli²⁹ proposed a calibration procedure of microscopic parameters in two-dimensional FDEM. Lei et al.³⁰ implemented an empirical joint constitutive model into FDEM to analyze the behavior of fractured rocks.

Recently, Yan et al.^{31–34} based on FDEM established two 2D/3D hydro-mechanical model (FDEM-flow2D/3D) to simulate fracturing driven by fluid. However, the method do not deal with problems of thermal cracking. Therefore, in this study we add a new feature to FDEM to simulate thermal cracking of rock, termed FDEM-TM. The organization of the paper is as follows. In Section 2, system equations and fracture criterion of joint element in FDEM are introduced briefly. Section 3 describes the coupled thermo-mechanical model, including thermal conduction model, thermal stress and the calculation processes of thermo-mechanical coupling, which is the core content of this paper. Finally, three examples with analytic solutions are given to verify the correctness of the coupled thermo-mechanical model to deal with problems of steady-state thermal conduction, unsteady-state thermal conduction and thermo-mechanical coupling, respectively. Moreover, a thermal cracking example is also given, and the simulation results of which are compared with experimental results.

2. Fundamentals of combined finite-discrete element method

In FDEM, the continuum in the problem domain is meshed into a finite element mesh composed by constant strain triangle (CST) elements, and joint elements with bonding effect are inserted in the

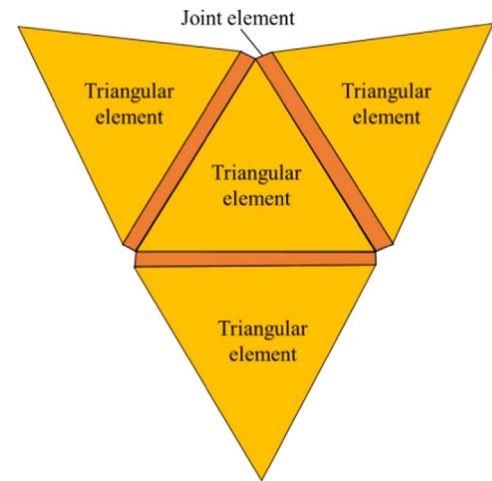


Fig. 1. Connection of triangular elements and joint elements.

common edge of adjacent triangular elements, as shown in Fig. 1. Thus, the triangular elements do not share nodes. Since the joint elements that connected two triangular elements may break and lost bonding effect, crack initiation, propagation and intersection can be simulated by the breakage of joint elements. While, before joint element broken, the continuum deformation can be represented by the triangular elements and joint elements with bonding effect.

2.1. System equations of FDEM

The dynamic equations of the system in FDEM are similar to that in discrete element method (DEM), given by

$$\mathbf{M}\ddot{\mathbf{x}} + \mathbf{C}\dot{\mathbf{x}} = \mathbf{F}(x) \quad (1)$$

where \mathbf{M} and \mathbf{C} are the mass matrix and damping matrix of nodes, respectively; $\mathbf{F}(x)$ represents unbalanced force vector of node, including the nodal force F_c caused by contact, the nodal force F_d by triangular element deformation, the nodal force F_e by the external load, and the nodal force F_j by bonding effect of joint element.

Since the statics problems are solved by dynamic relaxation method, the damping matrix \mathbf{C} is used to consume kinetic energy of system. Damping matrix \mathbf{C} is given by

$$\mathbf{C} = \mu \mathbf{I} \quad (2)$$

where μ is damping coefficient, \mathbf{I} is unit matrix. According to the mass spring system of single degree of freedom, the critical damping coefficient μ_c is given by

$$\mu_c = 2h\sqrt{\rho E} \quad (3)$$

where h is the edge length of element, ρ is density, E is elastic modulus. If critical damping coefficient μ_c is used, kinetic energy of system can be consumed with the fastest speed.

According to Eq. (1), in each time step, coordinates and velocity of a node can be calculated by central difference method, as the following formula

$$\begin{aligned} v_i^{(t+\Delta t)} &= v_i^{(t)} + \sum F_i^{(t)} \frac{\Delta t}{m_n} \\ x_i^{(t+\Delta t)} &= x_i^{(t)} + v_i^{(t)} \Delta t \end{aligned} \quad (4)$$

where $F_i^{(t)}$, represents the total nodal force, Δt is time step, m_n is node mass, which is equal to one third of a triangular element's mass.

2.2. Fracture criterion of joint element in FDEM

Since crack initiation and propagation are simulated by the breakage of joint elements in FDEM, the fracture criterion of joint element is vital to cracking simulation. In this section we introduce the fracture

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