Available online at www.sciencedirect.com
ScienceDirect
Trans. Nonferrous Met. Soc. China 25(2015) 2367−2379
Transactions of Nonferrous Metals Society of China
www.tnmsc.cn

Thermo-mechanical coupled particle model for rock

Ming XIA

Computational Geosciences Research Centre, Central South University, Changsha 410083, China

Received 10 March 2014; accepted 21 July 2014

Abstract: A thermo-mechanical coupled particle model for simulation of thermally-induced rock damage based on the particle simulation method was proposed. The simulation results of three verification examples, for which the analytical solutions are available, demonstrate the correctness and usefulness of the thermo-mechanical coupled particle model. This model is applied to simulating an application example with two cases: one is temperature-independent elastic modulus and strength, while the other is temperature-dependent elastic modulus and strength. The related simulation results demonstrate that microscopic crack initiation and propagation process with consideration of temperature-independent and temperature-dependent elastic modulus and strength are different and therefore, the corresponding macroscopic failure patterns of rock are also different. On the contrary, considering the temperature-dependent elastic modulus and strength has no or little effect on the heating conduction behavior. Numerical results, which are obtained by using the proposed model with temperature-dependent elastic modulus and strength, agree well with the experimental results. This also reveals that the rock subjected to heating experiences much more cracking than the rock subjected to cooling.

Key words: particle simulation method; micromechanics; rock fracture; thermo-mechanical coupled model

1 Introduction

With the characteristics of high strength, rock has been widely used in the engineering structure, such as tunnels, rock slopes, dams and petroleum reservoirs [1]. To ensure the safety and stability of these engineering structures, many researchers have studied its behaviors under mechanical condition during the past few decades. However, it is often under the thermo-mechanical coupled condition in many scientific and engineering fields. For example, in environment protection engineering, geological sequestration of CO_2 into deep saline aquifers could become a promising solution for reducing the CO_2 concentration in the atmosphere. In a deep aquifer, the injected CO_2 flow in the near-well injection zone can create a temperature gradient that leads to a macroscopic failure as a result of microscopic crack initiation, propagation, and coalescence in the surrounding rock mass. This implies that thermally-induced rock damage should be considered in simulating the behavior of near-well injection zone. Similarly, the geological isolation has been commonly adopted to dispose high-level radioactive wastes (HLW) produced from nuclear power stations. The radioactive heat generated by the decay of nuclear elements in the buried HLW can create a high temperature gradient around the surrounding rock mass. Due to the long half-life features of radioactive elements, the maximum temperature around surrounding rock mass can reach 200−300 °C [2]. To ensure the safety and stability of HLW repositories, it is necessary to consider thermally-induced rock damage on the 10^4−10^6 year time-scale. Although all the above mentioned problems may involve two or more processes, such as thermal, hydrological, mechanical and chemical processes (THMC), the focus of this work is mainly on the thermally-induced rock damage associated with thermal and mechanical coupling processes. Thus, a thermo-mechanical coupled model for rock, which can reproduce its mechanical and thermal behavior accurately, is of great significance for simulating the rock mechanical and thermal behavior under thermo-mechanical condition.

From the macromechanical point of view, the acoustic emission technology can be used to locate the microscopic acoustic emission source in rocks for

Foundation item: Project (41372338) supported by the National Natural Science Foundation of China
Corresponding author: Ming XIA ; Tel: +86-731-88830020; E-mail: xiaming105@126.com
DOI: 10.1016/S1003-6326(15)63852-3

monitoring thermally-induced rock damage. In particular, DONG and LI [3,4] optimized and simplified the sensor location coordinates to find the analytical solution of the acoustic emission source location coordinates. On the other hand, from the micromechanical point of view, the failure of rock under thermo-mechanical condition is governed by microscopic crack initiation and propagation. However, the continuum-based numerical methods, such as the finite element method and boundary element method, are difficult, if not impossible, to simulate the predominant mechanism of rock failure processes associated with microscopic crack initiation, propagation and coalescence [5]. In this way, a micromechanical model of rock based on the particle simulation method [6,7], which can track the initiation and propagation of mechanically-induced microscopic crack, has been proposed. XIA and ZHOU [8] used the model to simulate the rock failure process. ZHAO et al [9] used the model to study the effects of shear on solute retardation coefficient in rock fractures. ZHAO [10] studied the gouge particle evolution in a rock fracture undergoing shear. YOON et al [11] simulated the fracture and friction of Aue granite under compression using clumped particle model. Recently, XIA and ZHAO [12] simulated rock deformation and mechanical characteristics using clump parallel-bond models. Although these studies enhance the understanding of rock failure processes, they are concentrated on the mechanical field. As stated previously, rock is often under thermo-mechanical condition in some engineering problems. While in this work, the particle simulation method is extended from the mechanical field to thermo-mechanical coupling fields. It should be noted that a thermo-mechanical coupled particle model for rock has been proposed previously [13]. However, it has following two disadvantages: 1) the microscopic parameters of this model cannot be directly determined from the related macroscopic ones; 2) the temperature-dependent elastic modulus and strength are not considered. Furthermore, WANNE and YOUNG [14] used this model to simulate thermally fractured granite, but the microscopic crack initiation and propagation processes cannot be simulated at the cooling stage.

To overcome the above mentioned two disadvantages, a new thermo-mechanical coupled particle model for rock in the thermo-mechanical coupling system was proposed. For the purpose of verifying the proposed model for simulating the thermo-mechanical coupling problem, three examples, for which analytical solutions are available, were used to show the correctness and usefulness of the proposed model. Finally, an application example was simulated to investigate the thermally-induced rock damage using the present model with two different cases: one is temperature-independent elastic modulus and strength, while the other is temperature-dependent elastic modulus and strength.

2 Thermo-mechanical coupled particle model

Even though the details of the model and the related computational algorithms can be found in Ref. [15], for the sake of completeness of this work, only some key mathematical formulations of the thermo-mechanical coupling particle model based on the particle simulation method are briefly given below. In this model, rock material was simulated as an assembly of particles, which were connected to each other through their bonds in the case of simulating mechanical deformation, but connected to each other through thermal pipes in the case of simulating heat conduction.

Figure 1 shows the mathematical formulations used in the thermo-mechanical coupling simulation. In Fig. 1, the simulation of mechanical deformation is shown on the left side, while the simulation of heat conduction is shown on the right side. For the equation of motion, F_i is the resultant force exerted on the mass center of the particle; m is the mass of the particle; $\ddot{x}_i$ is the acceleration; g_i is the gravity acceleration; M_i is the rotation moment exerted on the mass center of the particle; I is the moment of inertia of the particle; $\ddot{\theta}_i$ is the angular acceleration. For the force−displacement equation, $F^{\mathrm{n}}_{\mathrm{mechanical}}(T)$ is the normal component of the temperature-dependent contact force; $K^{\mathrm{n}}(T)$ is the temperature-dependent secant normal stiffness; U^{n} is the normal displacement; $\Delta F^{\mathrm{s}}_{\mathrm{mechanical}}(T)$ is the incremental shear component of the temperature-dependent contact force; $k^{\mathrm{s}}(T)$ is the temperature-dependent tangential shear stiffness; ΔU^{s} is the incremental shear displacement. For the temperature calculation equation, T_t and $T_{t+\Delta t_{\mathrm{thermal}}}$ are the temperature at time t and $t+\Delta t_{\mathrm{thermal}}$, respectively; $\Delta t_{\mathrm{thermal}}$ is the thermal time step; c_V is the specific heat of the particle; $\widetilde{Q}$ is the out-of-balance heat power of the heat reservoir. For the heat flow calculation equation, Q^{p} is the heat power in pipe that is flowing out of the heat reservoir; ΔT^{p} is the temperature difference between the two heat reservoirs at the each end of pipe; and l^{p} is the length of pipe.

In the present model, a thermal pipe is associated with a specific contact. Once the thermal microscopic properties are assigned, subsequent loading or damage (in the form of bond breakages) will modify the number of active pipes, and thereby change the ability of the