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Modeling of coupled thermal-hydraulic-mechanical-chemical processes for predicting the evolution in permeability and reactive transport behavior within single rock fractures

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ABSTRACT

A multi-physics numerical model was developed to predict the fluid flow and mass transport behavior of rock fractures under coupled thermal-hydraulic-mechanical-chemical (THMC) conditions. In particular, the model was employed for the purpose of describing the evolution of permeability and reactive transport behavior within rock fractures by taking into account the geochemical processes of the free-face dissolution and the pressure dissolution. In order to examine the capability of the developed model, the model was applied to replicate the experimental measurements of the evolution in hydraulic aperture, permeability, and element concentrations obtained from two flow-through experiments using single granite and mudstone fractures. The model predictions for the granite experiment were able to follow the actual data for the evolution in hydraulic aperture and effluent element concentrations without adopting any fitting parameters that are often used in other THMC coupled models obtained from literature. Furthermore, the model succeeded in replicating the actual changes in fracture permeability and effluent element concentrations within the mudstone fracture. Although some uncertain mismatches between the experiments and the model predictions, such as changes in the concentrations of several elements (i.e., Na and K concentrations in the granite fracture and Al in the mudstone fracture) were remaining at this stage, the developed model should be valid for evaluating the evolution in the fluid flow and mass transport behavior within rock fractures induced by mineral dissolution under stress- and temperature-controlled conditions.

1. Introduction

Understanding the fluid flow behavior in the deep subsurface is essential for evaluating the performance of many rock engineering projects, such as the geological disposal of high-level radioactive waste[1–3] and anthropogenic CO_2,[4] and the enhanced geothermal system (EGS).[5] In the deep subsurface, the fluid flow behavior often depends on the hydraulic properties of the rock fractures (i.e., permeability and aperture) and the spatial distribution of the fracture network. It is well known that the permeability of fractured rocks is influenced by the coupled thermal-hydraulic-mechanical-chemical (THMC) processes under the deep geological conditions[6–8]. Among these several processes, mechanical-chemical (MC) processes, such as stress corrosion and geochemical reactions between the rock minerals and the pore water may exert a non-negligible influence on the evolution of fracture permeability[9–11]. However, within the context of the geological disposal of high-level radioactive waste, geochemical reactions, such as free-face dissolution/precipitation[12] and pressure dissolution[13–21], have been well recognized as important physical phenomena which may change the fracture permeability within a longer timescale in comparison to the mechanical processes. These processes within rock fractures have often been investigated under hydrothermal conditions where the fluid-rock reaction is enhanced.

Robert et al.[22] conducted flow-through column-like experiments for 20 and 40 days using granite samples with a single tensile fracture by simulating a near-field setting of the shallow Enhanced Geothermal System (EGS) (i.e., temperature of 120 °C and effective stress of 25–35 MPa), and the fracture permeability, the fracture aperture, and the mass of the dissolved minerals were computed through pore-pressure observations, effluent chemistry, and X-ray CT scan imaging, respectively. Their results showed the decrease in permeability that should have been due to a combination of the dissolution of the fracture

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propping asperities and mechanical creep. However, through measurements of the effluent solution, it was finally concluded that the decrease in permeability was actually due to the mineral dissolution of the fracture propping asperities rather than the mechanical effects. Beeler et al.[23] measured the time-dependent closure of fractures in quartz at temperatures of 22–530 °C and water pressures of 0.1–150 MPa, and reported a reduction in aperture of as much as 80% in just a few hours due to a pressure dissolution-like process. Besides these observations, many other experimental studies[9–11, 24, 25] have confirmed a reduction in the permeability of rock fractures by several orders of magnitude most likely brought about by the pressure dissolution.

Therefore, in order to predict the change in permeability of fractured rocks in actual fields, it should be of great importance to model the coupled THMC processes including the pressure dissolution. Conceptual models have been proposed in previous studies[9–11,16,18,24] to predict the evolution in permeability of porous and fractured rocks due to a mechanical-chemical phenomenon (i.e., pressure dissolution). These models can only describe the mechanical-chemical processes in the representative elementary scale; and thus, coupled THMC numerical simulations cannot be conducted with them at the field scale. The aim of this study is to propose an FE model that can describe the coupled THMC processes including the pressure dissolution for predicting the changes in rock permeability in the field scale. Previously, we developed a coupled THMC model using the FE scheme and incorporating the pressure dissolution at the grain-to-grain contacts[26]. Updating the model by incorporating the process of pressure dissolution at the contacting asperities is the main purpose of this study.

Recent studies[25,27–34] also have proposed several coupled THMC numerical models including the geochemical reactions (i.e., free-face dissolution and pressure dissolution) within rock fractures to estimate the evolution of fracture permeability. For instance, Lang et al.[27] developed a discrete multi-physics pore-scale model by extending the direct and coupled thermo-hydro-mechanical-chemical simulation approach of Bernabe et al.[28] from single, axisymmetric grain contacts to three-dimensional models of randomly rough, self-affine surfaces. The model can estimate the changes in fracture aperture induced by pressure dissolution and elastic compression. However, the focus of most of these studies[27–31] has only been the development of theoretical THMC models; the studies have not verified the developed models by comparing the predictions with actual measurements obtained from experiments.

In contrast, there are several studies[25,32–34] that have developed coupled models and examined their validity by a comparison with experimental data. Yasuhara et al.[25] developed a numerical model using the Lagrangian-Eulerian method that can predict the evolution of permeability and reactive transport behavior within a single novaculite fracture by describing the geochemical reactions (i.e., free-face dissolution and pressure dissolution). This model applied additional multipliers in the calculations of the mechanical-chemical processes in order to follow the experimental measurements – the multipliers ranged from 30 to 10^6. Based on the works by Yasuhara et al.[11,25], an attempt has been made to develop THMC numerical models that can reproduce the experimental measurements of single rock fractures using novaculite and granite[32–34]. In the scheme of their modeling, Bond et al.[33,34] applied some different modeling approaches, including the discretized 2D model that represents a 2D fracture surface taking the fracture topography data to locally define the fracture aperture, the homogenized (0D/1D/2D) model that treats the entire fracture surface as a single entity, and the synthetic model that uses the fracture topography data to define the statistics of the fracture aperture distribution. In these works[33,34], several participating teams attempted to apply these different modeling approaches with each team conducting calculations using their own numerical code. Most of different numerical models developed in their works[33,34] were able to replicate the experimental measurements relatively well (i.e., the evolution of fracture permeability and element concentrations), but in almost all cases, the prediction results were adjusted by incorporating fitting parameters, called enhancement factors and scaling factors, into the calculations of the mechanical-chemical processes with fitting parameters in the range of 245–10^6[32–34].

In this study, a new coupled-THMC model incorporating the pressure dissolution at the contacting asperities of rock fractures was developed using an FE scheme in order to predict the changes in permeability of rock fractures. As mentioned above, almost none of the other coupled THMC models[27–31], considering the pressure dissolution within rock fractures, have been validated and several coupled THMC models[25,32–34] need calibrations of the fitting parameters in wide ranges of 30–10^6[25] and 245–10^6[32–34] in the calculation of the mechanical-chemical processes in order to follow the experiments. This may not be the case for the model developed in this study – minimizing the use and the values of unknown, fitting parameters was a significant target for the model development. As is obvious, in order to examine the validity of the developed model, predictions made with the model were compared with the experimental measurements obtained from flow-through experiments[11] using granite and mudstone samples.

2. Model description

2.1. Constitutive equations

The coupled THMC model developed in this work is based on the finite element scheme that can describe the interactions of multi-physics that include the heat transfer, the fluid flow, geomechanics, and the reactive transport with the geochemical reactions of mineral dissolution/precipitation. By solving these THMC coupled processes, this model can evaluate the evolution of permeability in rock fractures. The equations for the model are presented in this section. The fluid flow in the fractures of saturated rock is simply modeled by the conservation of water mass and by assuming the Darcian flow, as follows:

$$\frac{\partial(\rho_w \phi)}{\partial t} + \nabla\cdot(\rho_w \mathbf{u}) = f_m, \tag{1}$$

$$\mathbf{u} = -\frac{\mathbf{k}}{\mu}(\nabla p + \rho_w g \nabla h), \tag{2}$$

$$k = \frac{b_h^2}{12}, \tag{3}$$

where ρ_w [kg m^{-3}] is the density of the fluid, ϕ [-] is the porosity, $\boldsymbol{u}$ [m s^{-1}] is the fluid velocity tensor, f_m [kg m^{-3} s^{-1}] is the source term for the flow, $\boldsymbol{k}$ [m^2] is the rock permeability tensor, μ [Pa s] is the fluid dynamic viscosity, p [Pa] is the fluid pressure, g [m s^{-2}] is the gravity acceleration, h [m] is the potential head, and b_h [m] is the hydraulic fracture aperture.

In the thermal process, the temperature of the rock is calculated by the heat transfer equation:

$$(\rho C_p)_{eq}\frac{\partial T}{\partial t} + \rho_w C_{p,w}\mathbf{u}\cdot\nabla T = \nabla\cdot(k_{eq}\nabla T) + Q_h, \tag{4}$$

where T [K] is the system temperature, $(\rho C_p)_{eq}$ [J K^{-1} m^{-3}] is the equilibrium volumetric heat capacity, $C_{p,w}$ [J kg^{-1} K^{-1}] is the heat capacity of the fluid, $\boldsymbol{k_{eq}}$ [W m^{-1} K^{-1}] is the equilibrium thermal conductivity tensor, and Q_h [W m^{-3}] is the heat source.

The mechanical behavior of rock structure is calculated by the quasi-static equilibrium equation and constitutive poroelasticity:

$$-\nabla\boldsymbol{\sigma} = \mathbf{F_v} \tag{5}$$

$$\boldsymbol{\sigma} = \mathbf{E}\colon(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon_T}) + \alpha_B P\mathbf{I} \tag{6}$$

where $\boldsymbol{\sigma}$ [Pa] is the stress tensor, $\mathbf{F_v}$ [Pa m^{-1}] is the body force, $\boldsymbol{E}$ [Pa] is the elasticity tensor, $\boldsymbol{\varepsilon}$ [-] is the strain tensor, $\boldsymbol{\varepsilon_T}$ [-] is the thermal strain tensor, α_B [-] is the Biot-Willis coefficient, and $\mathbf{I}$ [-] is the identity