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Coupled thermo-hydro-mechanical-chemical modeling by incorporating pressure solution for estimating the evolution of rock permeability

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ABSTRACT

A coupled THMC numerical model has been developed to examine the long-term change in permeability of the porous sedimentary rocks that are assumed to be composed purely of quartz. Specifically, the chemo-mechanical process of the pressure solution was incorporated into the model. The developed model was validated by replicating the existing experimental measurements of the porosity reduction and the evolving silica concentration. Subsequently, by simulating the burial of high-level radioactive wastes in the deep subsurface, namely, by applying the simulated confining pressure and temperature conditions, the long-term evolution of the rock permeability was predicted. The model predictions clearly showed a significant influence of the pressure dissolution on the change in permeability with time. The predicted permeability of the rocks close to the wastes decreased by one order of magnitude in 10^4 years when considering the pressure dissolution, while the permeability changed little during the same period when the pressure dissolution was not considered. This reduction should delay the dispersion of the radioactive materials dissolved in the groundwater.

1. Introduction

When disposing high-level radioactive wastes in the deep subsurface, the influence of the disposal on the hydraulic property of the rocks of interest must be examined in advance and should be estimated with a required precision. The rocks that work as natural barriers to the migration of radionuclides should be influenced by the convolved phenomena, including the transfer of heat from the wastes, the groundwater flow, the variation in induced stresses, and the geochemical reactions, such as mineral dissolution and precipitation.[1,2] Therefore, in order to predict the long-term evolution of the hydraulic property, a numerical model that can account for the coupled Thermo-Hydro-Mechanical-Chemical (THMC) processes is required. In particular, the precise modeling of the geochemical reactions, occurring at the interface between the grain particles composing the rocks and the pore water, is of significant importance to achieving precise predictions. To date, THMC numerical models have been developed to address such engineering issues as the geological isolation of CO_2 and radioactive wastes, and energy recovery from geothermal reservoirs.[3–9] By using some of the above models, the long-term phenomena taking place in the artificial and natural barriers have been predicted by considering the specific geological conditions, the heat transfer, the water flow, the stress/deformation, and the geochemical reactions. In the geochemical calculations of the THMC models, the mineral dissolution and precipitation occurring on the free surfaces of the rocks[10] are typically considered, but the dissolution active at the grain contacts (e.g., pressure dissolution[11–18]) is not taken into account. In our previous works,[19–23] it is indicated that the pressure dissolution may change the permeability of porous and fractured rocks by several orders of magnitude over a long duration; and therefore, the phenomenon must be incorporated into the modeling process when evaluating the long-term integrity of the rocks in terms of the hydraulic property. Recently, several THMC numerical models that can consider the process of the pressure dissolution have been proposed,[7–9] but these models mostly address fracture media and do not estimate the evolution of the hydraulic property within the matrix of porous rocks.

In this study, a new coupled THMC numerical model that incorporates the important process of the pressure dissolution, as well as the free-face dissolution and precipitation, was developed, and the validity of the model was examined by replicating the experimental measurements obtained from Elias and Hajash (1992).[24] Subsequently, the long-term evolution of the

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permeability in porous rock was predicted under the expected stress and temperature conditions where high-level radioactive wastes are disposed. In particular, the influence of the pressure dissolution on the change in the rock permeability was examined intensively.

When any numerical model is developed, it should be important to consider the balance between the simplicity and the precision of the model. Complex models that incorporate a number of equations to be solved may require time-consuming handling during pre- and post-processing, and lengthy calculation time. Therefore, simpler or more straightforward numerical models with satisfactory precision are preferred for general users. By focusing selectively on the geochemical process of the pressure dissolution, the minor objective of this study is to develop a relatively simple model.

2. Model description

The coupled THMC model developed in this work enables the change in permeability of porous rocks to be followed with time by considering the interactions of the thermal, hydraulic, mechanical and geochemical processes (i.e., heat transfer, groundwater flow in saturated porous media, stress/deformation, mass transport, and mineral dissolution/precipitation). The processes considered in this model are schematically summarized in Fig. 1. As is apparent from this figure, the two-way interactions are taken into account between the T and H, the H and C, and the C and T components. In the M component, the stress distribution is calculated and then rendered to calculate a chemo-mechanical process, which is referred to as CM in Fig. 1. In the C components, two different chemical processes are incorporated into the model; one is the free-surface dissolution/precipitation (CF) and the other is the pressure solution (CM). The pressure solution includes three serial processes - mineral dissolution at the stressed contacts, diffusive transport through the thin film of water, and re-precipitation of the mineral matter at the pore wall. The mineral dissolution at the stressed contacts is explicitly integrated into the proposed model as the CM component. It should be noted that we have proposed conceptual chemo-mechanical models to predict the change in permeability of porous and fractured rocks,[19–23] and that this work is an attempt to fit the conceptual model into the coupled numerical model and to conduct numerical simulations at a field scale instead of a representative element scale. It should be also noted that the interactions between the H and M and the M and T components are intentionally omitted in this work. These processes may influence the change in permeability, but the main focus of the current work is to examine the effects of the geochemical reactions (i.e., free-face dissolution/precipitation and pressure dissolution) on the change in permeability by simplifying the developed model.

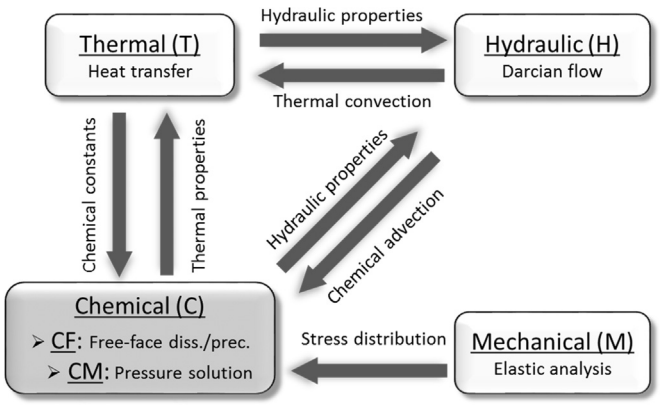

Fig. 1. THMC interactions considered in the developed numerical model.

2.1. Governing equations

The equations used to model each of the THMC processes are presented in this section. In this work, COMSOL Multiphysics[25] is utilized to solve the differential equations describing the THMC processes. The coupled THMC processes are solved sequentially by exchanging the dependent variables (i.e., porosity/permeability, flow velocity, stress, temperature, and dissolution/precipitation rate constants).

The groundwater flow in saturated rocks is simply modeled by the conservation of water mass and by assuming the Darcian flow, given by

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

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

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, and h [m] is the potential head. The temperature-dependent variables of ρ_w and μ are evaluated at arbitrary temperatures within the calculation scheme.[25]

The heat transfer is evaluated by considering thermal convection and conduction without the radiation effect, as follows:

$$(\rho C_p)_{eq}\frac{\partial T}{\partial t} + \rho_w C_{p,w}\,\mathbf{u}\cdot\nabla T = \nabla\cdot(\mathbf{k_{eq}}\nabla T) + Q_h, \tag{3}$$

where T [K] is the 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. $(\rho\, C_p)_{eq}$ and $\boldsymbol{k_{eq}}$ can be obtained from the following equations:

$$(\rho C_p)_{eq} = (1-\phi)\rho_m C_{p,m} + \phi\rho_w C_{p,w}, \tag{4}$$

$$\mathbf{k_{eq}} = (1-\phi)\mathbf{k_m} + \phi\mathbf{k_w}, \tag{5}$$

where ρ_m [kg m^{-3}] is the density of the solid, $C_{p,m}$ [J kg^{-1} K^{-1}] is the heat capacity of the solid, and $\boldsymbol{k_m}$ and $\boldsymbol{k_w}$ [W m^{-1} K^{-1}] are the thermal conductivity tensors of the solid and the fluid, respectively. The numerical model enables the temperature-dependent variables of $C_{p,m}$, $C_{p,w}$, $\boldsymbol{k_m}$, and $\boldsymbol{k_w}$ to be followed at arbitrary temperatures.[25]

The mechanical process of the rock structure is evaluated by the quasi-static equilibrium equation and the typical Hooke's law, given by

$$-\nabla\cdot\boldsymbol{\sigma} = \mathbf{F_v}, \tag{6}$$

$$\boldsymbol{\sigma} = \mathbf{E}\colon \varepsilon, \tag{7}$$

where σ [Pa] is the stress tensor, $\boldsymbol{F_v}$ [Pa m^{-1}] is the body force, $\boldsymbol{E}$ [Pa] is the elasticity tensor, and ε [−] is the strain tensor. In this work, the thermal stress and the inelastic behavior are disregarded for simplicity. A self-weight analysis is conducted to obtain the initial stress field, while the change in stress distribution by the cavity excavation is calculated using these equations.

The advection-diffusion equation is used to calculate the solute