A novel framework for coupled THMC analysis employing explicit rock fracture

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Abstract. A novel coupled thermal-hydraulic-mechanical-chemical (THMC) simulator for fractured porous rock was developed in the present study based on explicit fracture models. This work is an attempt to describe the spatial coupled phenomena sensitive to fracture generation within rock masses by using explicit fracture representation. The simulator was then applied to numerically predict the long-term evolution in the permeability of a rock mass working as a natural barrier within a geological disposal facility of high-level radioactive waste (HLW). The predicted results showed that the fractures generated due to the excavation of the disposal cavity drastically increased the rock permeability around the cavity and that the gradual decrease in permeability with time was caused only within specific fractures where the pressure solution had been activated after the disposal of the waste package into the cavity. The maximum decrease in permeability within the fractures was more than two orders of magnitude. Overall, it was confirmed that the developed simulator can capture the heterogeneous and local permeability evolutions among multiple fractures due to geochemical creep over the long term.

1. Introduction

When examining the performance of geological disposal facilities of high-level radioactive waste (HLW), it is essential to numerically predict the long-term evolution of the fracture permeability on the rock mass that works as a natural barrier. The fracturing within a natural barrier occurs due to the excavation of the cavity for disposing the HLW. Afterwards, the permeability of the generated fractures may be altered by the coupled phenomena among the fluid flow, earth pressure, solute transport, heat transfer, and geochemical reactions of the minerals and pore water. Therefore, both the fracture generation and the subsequent coupled thermal-hydraulic-mechanical-chemical (THMC) phenomena that may act on the rock fractures should be described reasonably. In particular, among the coupled phenomena, the geochemical reactions, such as the pressure dissolution at the contacting asperities within the rock fractures, may have a non-negligible influence on the change in fracture permeability with time over the long term [1]. Although many coupled simulators have been developed up to now [e.g., 2-4], most of them represent rock fractures based on continuum damage models and cannot explicitly capture the details of the formation of the fractures and the coupled phenomena acting on the fractures. Meanwhile, several coupled simulators based on explicit models of
rock fractures have also recently been proposed [e.g., 5-7]. Despite the fact that they are able to grasp the detailed phenomena related to rock fractures, including fracture initiation/propagation and various fluid-driven transport processes through the fracture network, the occurrence of geochemical reactions within the fractures have not been considered.

2. Description of simulator
In this study, a novel numerical simulator, which enables the depiction of the detailed responses of rock fractures, from their initiation/propagation to the subsequent coupled phenomena, including geochemical reactions (e.g., pressure solution), was developed based on explicit fracture models. Then, the developed simulator was applied to investigate the long-term change in the permeability of a rock mass that works as a natural barrier within a geological repository of HLW.

The numerical simulator developed in this work can address the change in rock permeability through fracture generation and subsequent restructuring, such as self-sealing/opening with time, by taking account of the multi-physics interactions among the heat transfer, groundwater flow, stress/deformation with the nucleation growth of the fractures, solute transport, and mineral dissolution/precipitation. These coupled interactions considered in the simulator are illustrated in figure 1. A two-dimensional natural barrier, composed of fully saturated porous rock, is the target of the numerical simulations in this study, while the phenomena in the artificial barrier are not considered. In the implementation system of the developed simulator, firstly, the fracture generation during the excavation of the disposal cavity is computed by the combined finite-discrete element method (FDEM) [8], which can explicitly reproduce the distinct fracture geometry. Each fracture obtained from the FDEM simulation in this work is expressed as a two-dimensional domain that reflects the fracture opening (i.e., fracture aperture). The simulation using FDEM is performed by an explicit time integration. Subsequently, after the disposal of the HLW into the cavity, the coupled phenomena controlled by the formation of fractures, including the fluid-driven transport processes and pore structure evolution within the fractures over time, due to geochemical reactions, are calculated by the discrete fracture network model (DFNM) based on an implicit time integration. In the DFNM simulation, each fracture is modelled as a one-dimensional element (i.e., line element) by converting the fracture geometry derived from the FDEM simulation. Constructing a reasonable numerical framework based on explicit fracture modelling to describe the spatial coupled phenomena sensitive to the newly generated fracture network within the rock mass is the most remarkable achievement of this study. On the other hand, it should also be noted that consideration of the change in stress/deformation with time after the disposal of the HLW is omitted in the simulator. This point will be addressed in a future study.

![Figure 1. Coupled THMC processes considered in simulator.](image)
2.1 Governing equations

The mechanical behaviour of the rock mass, including the fracturing process, is simulated by the FDEM. In the FDEM scheme applied in this work, the following dynamic equation for the nodes is solved by principals based on continuum mechanics, the intrinsic cohesive zone model, and contact mechanics. The open-source code, Y-code, developed by Munjiza [8], is used as the numerical tool for the FDEM.

\[
M \frac{\partial^2 \mathbf{u}}{\partial t^2} = f_{\text{ext}} + f_{\text{int}} + f_{\text{coh}} + f_{\text{con}}
\]  

(1)

where \( M \) [kg] is a lumped nodal mass, \( \mathbf{u} \) [m] is the nodal displacement, \( t \) [s] is the time, and \( f_{\text{ext}} \) [N], \( f_{\text{int}} \) [N], \( f_{\text{coh}} \) [N], and \( f_{\text{con}} \) [N] are the equivalent nodal forces corresponding to the external load, internal load, cohesive force, and contact force, respectively. \( f_{\text{int}} \) is computed by converting the Cauchy stress tensor which is expressed as equation (2).

\[
\sigma_{ij} = \frac{\lambda}{2} \left( J - 1 \right) \delta_{ij} + \frac{\mu}{J} \left( B_{ij} - \delta_{ij} \right) + \eta_{\text{coh}} d_{ij}
\]

(2)

where \( \sigma_{ij} \) [Pa] is the Cauchy stress tensor, \( B_{ij} \) is the left Cauchy-Green strain, \( \lambda \) [Pa] and \( \mu \) [Pa] are the Lame constants, \( J \) is the determinant of the deformation gradient, \( d_{ij} \) [s\(^{-1}\)] is the rate of the deformation tensor, and \( \eta_{\text{coh}} \) [kg m\(^{-1}\)s\(^{-1}\)] is the critical viscous damping coefficient. The rock fracturing is simulated by employing the intrinsic cohesive zone model. In this model, shown in Figure 2, cohesive elements, which are initially zero in thickness, are inserted between all adjacent triangular elements within the calculation domain, and the triangular elements are connected to each other by cohesive force. In order to reproduce the behaviour of the fracture process zone, the normal and shear cohesive tractions \( \sigma_{\text{coh}} \) and \( \tau_{\text{coh}} \) are altered by applying tensile and shear softening according to the opening and sliding displacements \((o \text{ and } s)\) (figure 2), respectively.

\[
\sigma_{\text{coh}} = \begin{cases} 
\frac{2o}{o_{\text{overlap}}} T_s & \text{if } o > 0 \\
\frac{2o}{o_p} \left( o \frac{o_{\text{overlap}}}{o_p} \right)^2 f(D_i) T_s & \text{if } 0 \leq o \leq o_p \\
f(D_i) T_s & \text{if } o_p < o 
\end{cases}
\]

(3)

\[
\tau_{\text{coh}} = \begin{cases} 
\frac{2s}{s_p} \left( s \frac{s_{\text{overlap}}}{s_p} \right)^2 \left( -\sigma_{\text{coh}} \tan(\phi) + f(D_2) c \right) & \text{if } 0 \leq s \leq s_p \\
-\sigma_{\text{coh}} \tan(\phi) + f(D_2) c & \text{if } s_p < s 
\end{cases}
\]

(4)

where \( o_p \) [m] and \( s_p \) [m] are the elastic limits of \( o \) and \( s \), respectively, \( \phi \) [°] is the internal friction angle of the cohesive elements, \( o_{\text{overlap}} \) [m] expresses the representative overlapping when \( o \) is negative, \( T_s \) [Pa] is the tensile strength of the cohesive elements, \( c \) [Pa] is the cohesion of the cohesive elements, \( D_i \) and \( D_2 \) are damage variables used for tensile softening and shear softening, respectively, and \( f \) is a function that affects the shape of the softening curve. In the model, positive \( o \) and \( \sigma_{\text{coh}} \) represent the crack opening and tensile cohesive traction, respectively. \( D_1 \) and \( D_2 \) are defined as follows:

\[
D_o = \min \left( 1, \frac{o - o_p}{o_t} \right) \quad \text{if } o_p < o, \quad \text{otherwise } 0
\]

(5)
where $D_o$ and $D_s$ are damage variables for the tension and shear modes, respectively, $\alpha_S$ is the constant which expresses the effect of the shear damage on tensile softening, and $D(0 \leq D \leq 1)$ is the damage variable that integrates the tensile damage and shear damage. $D$ becomes 0 when no damage occurs and 1 when complete damage occurs. In this study, a cohesive element ($D > 0.4$) is assumed as a “fracture”. In the current work, $\alpha_S$ in equation (7) is set to be 0.1 by assuming a partial link between the shear damage and the compactness of normal traction, while previous FDEM codes [e.g., 5,6,8] generally $\alpha_S$ set to 1.0. Generally, the behaviour of rock fracturing is affected by the heterogeneity of the natural rock mass. In this work, the heterogeneity of the rock mass is expressed by setting the mechanical properties ($T_s$ and $c$) of each cohesive element according to the Weibull distribution.

$$f(x) = \frac{m}{x_0} \left( \frac{x}{x_0} \right)^{m-1} \exp \left[ -\left( \frac{x}{x_0} \right)^m \right]$$

where $x$ is the mechanical parameter of the cohesive elements in the calculation domain, $x_0$ is the scale parameter, and $m$ is the homogeneity index of the mechanical properties.

The fluid-driven transport processes within porous rock after the fracturing process is computed based on the DFNM. Among them, equations only for the solute transport process are introduced in the following. In the scheme of the DFNM, different partial differential equations for the rock matrix zone and the fracture zone (fracture boundary is expressed by a line element) are solved together, and interactions between the two zones are also considered. From here, the rock matrix zone and the fracture zone are represented as $\Omega_m$ and $\Gamma_f$, respectively. The solute concentration in the pore water within the fractured rock is calculated by the following advection-diffusion equation, as

$$\frac{\partial(\phi C)}{\partial t} - \frac{k_m}{\nu} (\nabla p + \rho g) \cdot \nabla C + \nabla \cdot (D \nabla C) + \sum \frac{n}{i} \dot{V} R_i$$

in $\Omega_m$ (11)
\[
\frac{\partial (\phi c_i)}{\partial t} - \frac{k_f}{\nu} \nabla \cdot (\nabla \cdot c_i) = \nabla \cdot (D_{ij} \nabla c_i) + \sum_j \nu_j R_j \quad \text{in } \Gamma_f
\] (12)

\[
k_f = \frac{b^2}{12} \quad \text{in } \Gamma_f
\] (13)

where \(c_i \text{[mol m}^{-3}\]) is the concentration of solute \(i\), \(D_{ij} \text{[m}^2\text{s}^{-1}]\) is the effective diffusion coefficient tensor, \(\phi\) is the porosity, \(\rho_w \text{[kg m}^{-3}\]) is the water density, \(p \text{[Pa]}\) is the pore pressure, \(k_m \text{[m}^2\]) and \(k_f \text{[m}^2\]) are the rock permeability for the matrix and fracture zones, respectively, \(\nu \text{[Pa s]}\) is the water dynamic viscosity, \(g \text{[m s}^2\]) is the gravity acceleration, \(\nu_i\) is the stoichiometry coefficient of solute \(i\), \(n\) is the number of rock-forming minerals, \(R_j \text{[mol m}^{-3}\text{s}^{-1}]\) is the rate of geochemical reactions for mineral \(j\), \(Q_{c_i} \text{[kg m}^{-3}\text{s}^{-1}]\) is the supply of concentration of solute \(i\) from the rock matrix to the fracture space, \(\nabla\cdot\) expresses the spatial gradient in the tangential direction to the fracture plane, and \(b \text{[m]}\) is the fracture aperture.

In this work, the geochemical reactions between rock mineral and pore water include free-face dissolution/precipitation and the pressure solution. Thus, the rate of geochemical reactions for mineral \(j\), \(R_f\), is expressed as

\[
R_j = R_{jFF} + R_{jPS} \quad \text{in } \Omega_m \cup \Gamma_f
\] (14)

where \(R_{jFF} \text{[mol m}^{-3}\text{s}^{-1}]\) is the rate of free-face dissolution/precipitation of mineral \(j\) within the rock, and \(R_{jPS} \text{[mol m}^{-3}\text{s}^{-1}]\) is the rate of pressure solution of mineral \(j\) within the rock. Referring to Ogata et al. [9], the rate of the pressure solution within the fracture is formulated based on the geometric model by idealizing the arbitrary micro-domain as the representative element of fracture zone, as follows:

\[
R_{jPS} = \frac{3f_r \chi_p R V_{m,j} k_{v,j}}{RTb(1 - R_c)} \left( \frac{\sigma_n}{R_c} - \sigma_c \right) \quad \text{in } \Gamma_f
\] (15)

where \(f_r\) is the roughness factor, \(\chi_p\) is the volumetric ratio of mineral \(j\), \(R_c\) is the contact area ratio within the fracture, \(V_{m,j} \text{[m}^3\text{mol}^{-1}]\) is the molar volume of mineral \(j\), \(k_{v,j} \text{[mol m}^{-3}\text{s}^{-1}]\) is the mineral dissolution rate constant of mineral \(j\), \(\sigma_n \text{[Pa]}\) is the normal compressive stress that acts on the fracture plane, \(\sigma_c \text{[Pa]}\) is the critical stress, \(R \text{[mol m}^{-1}\text{K}^{-1}]\) is the gas constant, and \(T \text{[K]}\) is the system temperature.

The rock permeability is altered by updating the pore structure of the rock mass due to the fracture initiation/propagation and geochemical creep. Within the fracture zone, a change in aperture is considered a change in pore structure, while within the matrix zone, a change in porosity is considered a change in pore structure. The current work considers free-face dissolution/precipitation and pressure dissolution as geochemical reactions. Therefore, the fracture aperture at arbitrary time \(t\) is expressed by taking account of the aperture created by the fracturing process and the temporal evolution of the aperture induced by the free-face dissolution/precipitation and pressure dissolution, given as

\[
b(t) = b_D + b_{FF}(t) + b_{PS}(t) \quad \text{in } \Gamma_f
\] (16)

\[
b_{FF}(t) = \left[ \sum_j 2 f_r \chi_p (1 - R_c) V_{m,j} k_{v,j} \left( 1 - \frac{Q_j}{K_{eq,j}} \right) \right] dt \quad \text{in } \Gamma_f
\] (17)

\[
b_{PS}(t) = \left[ \sum_j \frac{3f_r \chi_p V_{m,j} k_{v,j}}{RT} \left( \frac{\sigma_n}{R_c} - \sigma_c \right) \right] dt \quad \text{in } \Gamma_f
\] (18)
where \( b_0 \) [m] is the aperture generated by the fracturing process, which is equivalent to the fracture opening obtained from the FDEM simulation, \( b^{eff}(t) \) [m s\(^{-1}\)] is the rate of change in the fracture aperture by free-face dissolution/precipitation, \( b^{qs}(t) \) [m s\(^{-1}\)] is the rate of change in the fracture aperture by pressure dissolution, \( Q_{j} \) is the ion activity product of mineral \( j \), and \( K_{eq,j} \) is the equilibrium constant of mineral \( j \). Equations (17) and (18) are based on Ogata et al. [9]. When the fracture aperture changes, the contact area also changes. This relationship is given by the following equation:

\[
b(t) = b_r + (b_0 - b_r) \exp \left( \frac{R_{c,D}(t) - R_{c,D}}{a} \right)
\]

in \( \Gamma_f \) (19)

where \( b_r \) [m] is the residual fracture aperture, \( R_{c,D} \) is the contact area ratio within the fracture when a fracture is generated, and \( a \) is a constant. \( R_{c,D} \) is computed based on the Hertzian contact theory [10] by assuming that the asperity contacts within fractures are microscopic grain contacts.

\[
R_{c,D} = \left( \frac{3\sigma \pi (1-\nu^2)}{4E} \right)^{\frac{2}{3}}
\]

in \( \Gamma_f \) (20)

where \( \nu \) is Poisson’s ratio and \( E \) [Pa] is the elastic modulus of the rock mass.

### 3. Numerical simulation for long-term prediction

The developed simulator was utilized to examine the long-term evolution of the permeability in a natural barrier with a geological disposal facility of HLW under virtual subsurface conditions. Notably, although actual data from related literature were used in the following simulations, no specific site for the HLW disposal facility was assumed.

The numerical domain represented fully saturated sedimentary rock that was composed purely of quartz at a depth of 300 m to 400 m from the Earth’s surface, with a disposal cavity having a diameter of 2.0 m and a depth of 350 m. The horizontal length of the numerical domain was 20 m. In this numerical prediction, firstly, an excavation analysis of the disposal cavity was performed, and secondly, a long-term coupled simulation was conducted. The saturated density of the target rock was 2640 kg/m\(^3\) [11]. The initial porosity and permeability were set to be 0.416 and 2.88×10\(^{-16}\) m\(^2\), respectively [11]. The characteristic values for the Weibull distribution of the tensile strength and cohesion were 2.38 MPa and 4.33 MPa, respectively. The hydraulic and thermal gradients were set to be 1/1000 and 5 °C/100 m, respectively [12]. The surface temperature was fixed at 15 °C. The homogeneity index of the Weibull distribution was set to 3.0. The elastic modulus, Poisson’s ratio, and internal friction angle were 1.82 GPa, 0.17, and 26°, respectively. In the excavation analysis, the mechanical response of the rock mass was computed using the FDEM, including the fracturing process during the excavation of the disposal cavity with a diameter of 2.0 m. The lateral earth

![Figure 3](image)

**Figure 3.** Fracturing due to excavation: (a) fracture formation after excavation, (b) damage mode of fractures, and (c) permeability distribution after excavation.
pressure coefficient was set to be 0.95 [11]. The fracture generation (distribution of damage variables $D$, damage mode, and permeability distribution around the disposal cavity after the excavation are shown in figure 3. In figure 3(b), the tension mode (only tensile damage) and shear mode (only shear damage) are expressed as areas of blue and red, respectively, and the mixed mode (tensile damage and shear damage) is depicted as areas of green. In figure 3(c), the permeability is shown by log notation (i.e., $\log_{10}(k)$). The figures show that multiple cracks were generated around the cavity, that rock permeability drastically increased in the fractured zone, and that the damage induced only by the shear mode was the most prominent. The maximum crack extension is 1.5 m (0.75 times the cavity diameter) from the cavity and the most easily observed change in permeability due to fracturing is an increase of about three orders of magnitude. The fracture properties (formation, distribution of aperture, and contact area ratio) and distribution of normal stress acting on the fractures when excavation was completed, were set as the initial conditions of the subsequent long-term simulation. The simulation period was designated to be $10^3$ years after the disposal of the HLW into the cavity. In this simulation, the change in the stress condition was not considered. The time-dependent temperature history was set at the periphery of the cavity as the boundary condition in order to consider the heat radiation from the waste package. This long-term coupled analysis was computed with the DFNM.

In the current work, the long-term simulations were performed for two different cases. The case that considers the coupled processes with pressure dissolution is called the “PS condition”. The other case that does not consider the pressure dissolution process is called the “no-PS condition”. The alterations in fracture permeability around the disposal cavity under the no-PS and PS conditions are shown in figure 4. In the figure, the permeability that is normalized by the initial value is shown by log notation (i.e., $\log_{10}(k/k_0$)). As is apparent from the figure, the permeability in several fractures irregularly decreased with time under the PS condition, while the permeability in almost all the fractures changed only a little over time under the no-PS condition. This decrease in permeability is attributed to the occurrence of the pressure solution at the asperity contacts within the fractures that depends on the heterogeneous properties of each fracture, such as the geometrical formation, aperture, closing stress, and contact area ratio. Based on equation (18), the pressure solution occurred only within the fractures where the compressive stress at an asperity contact ($\sigma_n/R_c$) was over the critical stress ($\sigma_{c}$). In the fractures where the pressure solution was induced most significantly, the permeability was eventually reduced to $10^{-2.5}$ times the initial value of the long-term simulation over the $10^3$ years.
4. Conclusion
A novel coupled numerical simulator, based on explicit fracture models, was proposed. The simulator can consider even the long-term change in permeability due to geochemical reactions. Then, the proposed simulator was applied to predict the long-term change in permeability of sedimentary rock that works as a natural barrier for a geological repository of HLW. The predictions revealed that rock fracturing due to the excavation of the disposal cavity resulted in a significant increase in permeability around the cavity and, after the excavation, the permeability only in several fractures where the pressure solution at the asperity contacts had been activated, gradually decreased with time over the long term. The occurrence of the pressure solution was controlled by the unique properties of each fracture (formation, aperture, closing stress, and contact area). Overall, the predicted results imply that the simulator developed in this work may be able to track the actual change in heterogeneous permeability during the disposal period of HLW due to geochemical creep by resolving the spatial distribution of the above-mentioned fracture properties in detail using explicit fracture representation.

Acknowledgements
This work was supported by JSPS KAKENHI, subject nos. 20K14826. Th support is gratefully acknowledged.

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