Micromechanical thermo-hydro-mechanical coupled model for fractured rocks considering multi-scale structures and its engineering application

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Abstract. Most existing studies on the coupled thermal-hydro-mechanical models for fractured rock mass are formulated using the macroscopic phenomenology method. As a result, the micromechanical behaviors of discontinuities, which essentially control the macroscopic response of the material, are not well considered in modeling the thermal-hydro-mechanical coupling processes for disturbed rock mass. In this study, the fractured rock mass is characterized by an anisotropic medium containing arbitrarily distributed penny-shaped microcracks in rock blocks separated by multiple sets of critically orientated fractures of large scales. This is an anisotropic coupled thermal-hydro-mechanical model for deformed saturated rock masses, which is capable of considering the alteration of macro-meso discontinuities. A multiscale damage constitutive model for fractured rock mass with the thermal-hydro-mechanical coupling is presented based on the Mori-Tanaka homogenization method and the thermodynamics theory. The influences of anisotropic damage growth, sliding dilatancy and normal compression of small-scale microcracks, and shear sliding and mobilized degradation of large-scale fractures are commendably accounted for. To reflect the anisotropic strength, the interaction between large-scale fractures and small-scale microcracks is also considered by practically relating the microcracks damage resistance to the orientation of fractures. By capturing the deformation of fractures and the opening and connectivity variations of microcracks with the constitutive model, the multi-scale structural change-induced permeability variation is modeled by the volumetric averaging method. The constitutive model and permeability tensor formulation have been implemented in a FEM code, which is then coupled with the well-established non-isothermal fluid flow simulator TOUGHREACT by an interlaced algorithm to establish a coupled thermal-hydro-mechanical numerical simulation platform. A numerical example is finally performed to investigate the effects of multi-scale structures and thermal-hydro-mechanical couplings on the water injection-induced temperature, pressure, and deformation responses of a deeply buried geothermal reservoir. The research may provide a useful reference for deepening the study of the thermal-hydro-mechanical couplings in deep rocks.

1. Introduction
The modeling requirements of complex couplings between the thermal (T), hydrological (H) and mechanical (M) processes in fractured rocks are vital for the performance assessment in various areas of deeply engineering activities, such as geothermal resources exploitations, hydropower engineering, CO₂ geologic sequestrations, nuclear waste disposals, etc. The deeply buried fractured rocks are typically characterized by high geotemperature, high pore fluid pressure and high geostress. Under
engineering disturbances, like reservoir stimulations, tunnel excavations or energy productions, the surrounding rocks may suffer a great perturbation. As a result, variations of rock stresses, fluid flow and heat transfer occur, and rock deformations happen simultaneously. Therefore, the engineering disturbance-induced T-H-M coupling processes occur around the disturbed rock mass. The coupled T-H-M effect may cause variations in the geometries (opening, size, connectivity, etc) of internal void system, usually comprised of large-scale fractures and small-scale microcracks/pores, which essentially control the transmission characteristics and coupling properties of fractured rocks. As the micro/macro void structures change, the deformation and transmission behaviors of fractured rocks vary accordingly. Meanwhile, the microscope structures may play a comparable effect on the T-H-M responses when compared with the macroscopic structures in the deep-seated rock mass. Thus, it’s of importance to develop the T-H-M coupled model accounting for different scales of void structures.

In this paper, the effect of multi-scale structures of fractured rocks on their coupled T-H-M process around the disturbed rock mass of deeply-buried engineering. The fractured rocks are characterized by an equivalent anisotropic medium containing various sizes of rock blocks separated by large-scale fractures, in which arbitrarily distributed penny-shaped small-scale microcracks are distributed in the rock blocks. In consideration that the large-scale fractures are usually clustered in several critical orientations affected by formation history and geological modes in practice, one or multiple sets of parallel fractures are reasonably considered in the fractured rocks. Starting from the multi-scale structures of fractured rocks, a micromechanical-based equivalent model under T-H-M coupled loading is presented in consideration of the influences of microcracks growth, opening and closing and fractures deformation and degradation on the mechanical behavior. By characterizing the variations in the geometries of microcracks and fractures system, the scale-dependent and deformation-dependent permeability tensor is given in accounting of the coupled T-H-M effect. A coupled T-H-M model is established via combining the mechanical model with the fluid flow and heat transfer modeling code, TOUGHREACT. This study differs from the existing researches on T-H-M coupling analysis in the consideration of macro-meso structures, rather than only microcracks or macroscopic fractures accounting (Rutqvist et al. 2002; Chen et al. 2013, Lee et al. 2020), thus exhibiting an advantage in including multi-scale structures in coupled T-H-M modeling.

2. Formulation of a T-H-M coupled model

From the multi-scale perspective, the representative volume element (RVE) is considered as an equivalent continuum containing various shape and size of rock blocks divided by \( n_J \) sets of parallel, planar and persistent large-scale fractures at the macroscopic scale, while at the microscopic scale \( n_r \) sets of penny-shaped small-scale microcracks are assumed to be arbitrarily distributed in the solid matrix of rock blocks. Under T-H-M coupled loading, the global responses of the fractured rock mass come from both large-scale fractures and small-scale microcracks.

2.1. A micromechanical-based damage constitutive model

In the T-H-M coupling frame, the fractured rock mass is assumed to be applied with a uniform macroscopic stress field \( \Sigma \) and saturated with a fluid pressure \( p \), while its temperature is heated to \( T \) from \( T_0 \). The global strain of the fractured rock mass is comprised of the strain of solid matrix, microcracks system and fractures system and the thermal strain:

\[
E = E^s + \sum_{r=1}^{n_r} E^r + E^T + \sum_{J=1}^{n_J} E^J
\]

(1)

where \( E, E^T, E^r, E^J \) are the total strain, the thermal strain, the strain of rock matrix, the strain of \( r \)th set of microcracks and the strain of \( J \)th set of fractures. \( E^T = \alpha T(T - T_0) \), \( \alpha \) is the thermal expansion tensor, for isotropic case \( \alpha = \alpha \delta \), \( \delta \) represents the Kronecker delta tensor. \( E^r = \beta (n^r) \otimes n^r + \gamma (n^r) \otimes n^r \), \( \beta (n^r) \) and \( \gamma (n^r) \) are two internal variables characterizing volume-average opening and sliding of the \( r \)th set microcracks, \( n^r \) denotes the unit normal direction.
At the macroscopic scale, the traction continuity when crossing planar fractures indicates that the macroscopic stress tensor of rock blocks and fractures equals the uniform macroscopic stress field $\Sigma$. Assuming the rock blocks and the fractures are fully saturated, the effective macroscopic stress $\Sigma'$ is

$$\Sigma' = \Sigma + pb\delta$$

where $b$ is the macroscopic isotropic Biot coefficient for the fractured rock mass.

Using an elasto-plastic model with the effective stress $\Sigma'$ to characterize the macroscopic mechanical behavior of a single fracture with the unit normal vector of $n'$, the displacement jump $g$ comprising of the elastic part $g^e$ and the plastic part $g^p$ is expressed as

$$g = g^e + g^p, \quad g^e = \left(\mathbf{H}'\right)^{-1} \cdot \Sigma' \cdot n' = \left(\mathbf{H}'\right)^{-1} \cdot \left(\Sigma \cdot n' + pbn'\right)$$

where $\mathbf{H}'$ represents the second-order elastic stiffness tensor of the $J$th set of fractures. Assuming the normal and tangential stiffnesses are $H_n$ and $H_t$, then $\mathbf{H}' = H_t (\delta - n' \otimes n') + H_n n' \otimes n'$. The plastic displacement jump $g^p$ is modeled by the classical saw-tooth model with an asperity angle $\alpha$, whose value can be determined considering the multi-order asperities (Liu et al. 2016). The yield function $F'$ and the slip potential $Q'$ utilized to control the shear slipping and dilatancy behaviors of the fracture are established on the asperity surface at an angle of $\alpha$, and the expressions are as follow

$$F' = \sigma_n'^i \sin \alpha + \left(\sigma_t'^j - c^j\right) \cos \alpha + \mu \left[\sigma_n'^i \cos \alpha - \left(\sigma_t'^j - c^j\right) \sin \alpha\right]$$

$$Q' = \sigma_n'^i \sin \alpha + \sigma_t'^j \cos \alpha$$

where $\sigma_t'^j$ and $\sigma_n'^i$ are the macroscopic effective shear and normal tractions action on the planar fracture with the unit normal vector of $n'$. $\mu$ and $c$ are the friction coefficient and cohesion of the fracture. From Eq. (4b), one can find that the dilatancy of the fracture is closely related to the asperity angle. To consider the decaying process of fracture dilatancy due to asperities abrasion and damage during shearing, the asperity angle $\alpha$ could decay with the accumulation of plastic tangential energy $W^p_t$

$$\alpha = \alpha^{peak} \exp(-\sigma'^i W^p_t)$$

For the $J$th set of fractures, let $s^r$ represents the average spacing, then its macroscopic strain, $E^J$, can be obtained with the displacement jump $g$ by the divergence theorem:

$$E^J = E^k + E^b = \frac{1}{s} g^e \otimes n'$$

where $E^k$ and $E^b$ denote the elastic and plastic parts of $E^J$.
adopted in this study. Using the microscopic damage variable $d$ to characterize the microcrack density,

$$d = N \cdot a,$$

in which $N$ represents the number of microcracks per unit volume, $a$ denotes the average radius. The opening and sliding of microcracks are described by the two above-mentioned volume-average internal variables $\beta(n')$ and $\gamma(n')$. The evolutions of the internal variables $d$, $\beta(n')$ and $\gamma(n')$ are given under the framework of thermodynamics.

The free enthalpy of the fractured rocks is composed of the free enthalpies of $n_J$ sets of persistent fractures and cracked rock blocks, which are cutting by $n_r$ sets of penny-shaped microcracks. Since the main effect of temperature change under T-H-M coupled loading is often realized by the induced thermal stress, the effects of thermal creep and direct couplings between temperature $T$ and damage $d$ and plastic strain $E^p$ are neglected. Considering the formulation of free enthalpy for layered rocks provided by Liu et al. (2021) using the Eshelby solution-based two-step homogenization procedure and the thermal effect-induced energy function proposed by Stabler and Baker (2000), the free enthalpy of saturated fractured rocks containing both large-scale fractures and small-scale microcracks under T-H-M coupled condition is given as below:

$$W^* = \frac{1}{2} \left( \Sigma + pb \delta \right) : S^* : (\Sigma + pb \delta) + \left( \Sigma + p \psi \right) - \sum_{j=1}^{n_J} \int \frac{H_{J}}{2d} \beta^J(n') + \frac{H_{J'}}{2d} \gamma^J(n') \cdot \gamma(n') \right] + \frac{p^2}{2N} + E^r : \Sigma \right.

$$

$$+ \frac{E^r : \mathcal{C}^r : E^r}{2} - c^r \left[ T - T_0 - T \ln \left( \frac{T}{T_0} \right) \right] + \sum_{j=1}^{n_J} \int \left[ n^J - (\Sigma + pb \delta) \cdot \left( H^J \right)^{-1} \cdot \left( \Sigma + pb \delta \right) \cdot n^J \right]$$

$$+ E^r : (\Sigma + pb \delta)$$

where $S^*$ represents the fourth-order isotropic elastic compliance tensor of the rock matrix, which is determined with its Poisson’s ratio $v^r$ and Young’s modulus $E^r$; $c^r$ is specific heat of the fractured rocks; $\mathcal{C}^r$ denotes the fourth-order equivalent elastic stiffness tensor of the fractured rocks, $\mathcal{C}^r = \left[ S^* + \sum_{j=1}^{n_J} \frac{1}{s^J} n^J \otimes \left( H^J \right)^{-1} \otimes n^J \right]^{-1}$. Note that during the formulation of Eq. (7), an isotropic Biot coefficient tensor of cracked rock blocks is adopted for simplification due to the arbitrary distribution of microcracks. $N$ denotes the Biot modulus of cracked rock blocks, $N = E^r / [3(1 - 2v^r)(b - \phi_b^e)]$, $\phi_b^e$ is the initial porosity for rock blocks.

From the state law of thermodynamics, the total strain of saturated fractured rocks under T-H-M condition can be obtained by partial derivation of the free enthalpy shown in Eq. (7) to $\Sigma$. Comparing the expression of $\partial W^* / \partial \Sigma$ with Eq. (1), the macroscopic strain of rock matrix, $E^r$, is provided

$$E^r = \frac{\partial W^*}{\partial \Sigma} = S^* : (\Sigma + pb \delta)$$

From Eqs. (1), (6) and (8), the expression of macroscopic stress described with the macroscopic strain is given as below:

$$\Sigma = \mathcal{C}^r : (E - E^T - \sum_{j=1}^{n_J} E^J - \sum_{j=1}^{n_J} E^{p,J} - S^* : pb \delta - \sum_{j=1}^{n_J} \frac{pb}{s^J} n^J \otimes n^J)$$

Evolution of the RVE porosity, $\phi$, is obtained by partial derivation of the free enthalpy to $p$:

$$\phi - \phi_b = \frac{b \delta : E^r + \delta : E^r}{N} + \frac{P}{N} + b \sum_{j=1}^{n_J} \delta : E^r$$

From Eqs. (9) and (10), one can find that the influences of both small-scale microcracks and large-scale fractures on the macroscopic stress-strain relation and porosity evolution of fractured rocks are well characterized.
Based on the free enthalpy shown in Eq. (7), the thermodynamic forces, $F^\beta$, $F^\gamma$ and $F^r$ conjugated to the internal variables $d$, $\beta(n')$ and $\gamma(n')$ for the $r$th set of microcracks can be determined from the partial derivation of the free enthalpy to each variable:

$$F^\beta(n') = \left[ \frac{H_o}{2d} \beta(n') + \frac{H_o}{2d} \gamma(n') \cdot \gamma(n') \right]$$  (11a)

$$F^\gamma(n') = \Sigma : n' \otimes n' - \frac{H_o}{d} \beta(n') + p$$  (11b)

$$F^r(n') = n' \cdot \Sigma : (\delta - n' \otimes n') - \frac{H_o}{d} \gamma(n')$$  (11c)

Evolutions of $\beta(n')$ and $\gamma(n')$ are given in two cases: opening state and closing state of microcracks. In the opening state, $\beta(n')$ and $\gamma(n')$ can be simply calculated by the conditions that $F^\beta(n') = 0$ and $F^\gamma(n') = 0$. For the closing state of microcracks, $F^\beta(n') < 0$, the effects of microcrack compressive closure and shear dilatancy are accounted. Normal compressive deformation of closed microcracks is modeled by a hyperbolic function, $\beta = F^\beta \beta_0 / (k_0 \beta_0 - F^\beta)$, $\beta_0$ and $k_0$ denote the initial closure and normal stiffness. Shear dilatancy of closed microcracks is modeled by associative Mohr-Coulomb criterion, $F = F^\gamma | + \mu F^\beta$, $\mu$ represents the friction coefficient. Evolution of $d$ is characterized by the yield criterion expressed below:

$$f(F^d, d) = F^d - V(d) = F^d - V(d_c) \frac{2d / d_c}{1 + (d / d_c)^2}$$  (12)

where $V(d)$ denotes the microcrack propagation resistance and attains its maximum value, $V(d_c)$, at the critical damage $d_c$. The first increasing then decreasing form of $V(d)$ can well model the damage softening.

The interaction between small-scale microcracks and large-scale fractures may play an important effect on the anisotropic strength of fractured rocks. In this study, the complex interaction is practically considered by relating $V(d)$ to the orientation of microcracks and fractures:

$$V(d_c) = V_0 \prod_j (\theta + (1 - \theta) \frac{2\kappa_j}{1 + \kappa_j^2})$$  (13)

where $\kappa = 1 \cdot |n' \cdot n'|$; $V_0$ and $\theta$ are introduced parameters to characterize microcrack-fracture interaction. Eq. (12) shows that microcracks in the orientation close to fractures tend to easily growth.

2.2. Structure-dependent permeability tensor

The equivalent permeability of fractured rocks contains the contribution from rock matrix, microcracks and fractures. Under T-H-M coupled loading, variations of the microcracks and fractures systems are modeled by the mechanical model mentioned above and characterized by the variables $\beta(n')$, $\gamma(n')$, $d$ and $g$. Using Poiseuille’s law describes the flow through microcracks and fractures, the permeability tensor of fractured rocks is calculated by the volume-average method:

$$K = (1 - \phi) k^r \delta + \sum_{i=1}^n k_0^i \left( \frac{d}{d_0} \right)^{x-3} \frac{\beta_0^3}{\beta_0} (\delta - n' \otimes n') + \sum_{j=1}^n k_j^f \left( \frac{b_j}{b_0} \right)^3 \frac{b_j}{s} (\delta - n' \otimes n')$$  (14)

where $k^r$ is the permeability of rock matrix; $k_0^i$ denotes the permeability of microcracks with initial volume fraction $\beta_0$ and density $d_0$; $k_j^f$ represents the permeability of a single fracture with initial
aperture $b'_0$, while $b'$ denotes the current aperture, $b' = b'_0 + \mathbf{E} : \mathbf{\delta}$. From Eq. (14), one can find the significant implications shown below:

1. Variation in $K$ under T-H-M loading is caused by both the damage growth of microcracks and deformation of fractures. This well considers the effects of multi-scale structures.
2. $K$ is of dependence on the geometries of microcracks and fractures system, rather than on stresses. This is more scientific and could integrate the post-peak strain-softening behavior.
3. The orientations of both microcracks and fractures could render the anisotropy of $K$.
4. During the implementation of a finite element code, a different $K$ could be associated with each geological domain or each group of elements, as long as the geometries parameters of microcracks and fractures for the subdomains or elements could be evaluated beforehand.

3. Computation approach

The proposed constitutive and permeability model presented in Eqs. (9), (10) and Eq. (14) have been integrated into the previously developed H-M coupled code (Liu et al. 2021), which had integrated the finite element method-based mechanical code and the well-established open-source code, TOUGHREACT. The control equations for saturated flow and thermal transfer are shown below:

\[
\frac{\partial}{\partial t} \left( \phi \rho_i X^e_i \right) = q_c - \nabla \left[ -\rho_i X^e_i \frac{K}{\mu} \nabla p + \rho_i g \right]
\]

\[
\frac{\partial}{\partial t} \left( (1 - \phi) \rho_e c^T \phi \rho_i \mu_i \right) = q_h - \nabla \left[ -\lambda_e \nabla T + \frac{h_i}{\mu_i} \frac{K}{\mu} \nabla p + \rho_i g \right]
\]

where $\rho_i$ and $\rho_e$ denote the density of fluid and rock grain; $\mu$ is the viscosity; $\lambda_e$ is the thermal conductivity.

The T-H-M coupled problem is solved sequentially by an interlaced algorithm: at each time step, fluid pressure $p$ and temperature $T$ are solved first by TOUGHREACT, then the mechanical process is handled to obtain the deformations of microcracks and fractures, the permeability and porosity of fractured rocks are finally updated and fed back into TOUGHREACT for next step calculation.

4. Simulation study

In this section, the coupled T-H-M process of the Rittershoffen geothermal project in Northern Alsace, France is investigated. Two geothermal wells had been drilled to extract the heat source at the target depth of 2.2~2.4km. To enhance the injectivity of injection well, a stimulated zone obtained by thermal-chemical-hydraulic (TCH) stimulations is 300m in length (Vidal et al. 2017).
The numerical calculation model is shown in Figure 1, four material zones are considered, a lower sediment layer, an upper granite layer, a TCH stimulated zone and a highly permeable zone. The quasi-3D finite element grid is densely distributed near the two wells and sparse far away, with a total of 625 brick elements and 1324 nodes. Both large and small structures are considered in the stimulation zone: two sets of large-scale orthogonal vertical fractures and randomly-distributed small-scale microcracks. The Biot coefficient is 0.6, specific heat is 800 $\text{J/kg/K}$, volumetric thermal expansion is $1.4 \times 10^{-5} \text{K}^{-1}$. Except for the parameters given in Table 1, other parameters for fractures and microcracks are showing below:

\[
\begin{align*}
  b_0 &= 0.1 \text{mm}, \\
  \alpha &= 10^\circ, \\
  H_N &= 100 \text{MPa/mm}, \\
  H_T &= 100 \text{MPa/mm}, \\
  \mu' &= 0.58, \\
  k_0 &= 8.0 \times 10^{-11} \text{m}^2; \\
  \beta_0 &= 0.01, \\
  k_0' &= 3 \text{GPa}, \\
  c_\mu &= 0.7.
\end{align*}
\]

| Table 1. Simulation parameters of the four considered materials in the study. |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Parameter       | TCH stimulated zone | Lower sediment layer | Upper granite layer | Highly permeable zone |
| $E_s$ (GPa)     | 20.0             | 15.0             | 25.0             | 20.0             |
| $\nu$           | 0.25             | 0.23             | 0.25             | 0.25             |
| $\lambda_m$ (Wm$^{-1}$K$^{-1}$) | 3.1             | 1.4             | 3.1             | 3.1             |
| $\phi$          | 0.06             | 0.09             | 0.03             | 0.06             |
| $k_s$ (m$^2$)   | $1.1 \times 10^{-15}$ | $1.1 \times 10^{-15}$ | $1.1 \times 10^{-15}$ | $1.6 \times 10^{-14}$ |

| Table 2. Lists of simulations, with differences of considered structures and fracture spacings. |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Simulations     | Case 1          | Case 2          | Case 3          | Case 4          | Case 5          |
| Considered      | fractures       | microcracks     | fractures+      | microcracks     | fractures+      |
| structures      | fractures       | microcracks     | microcracks     | microcracks     | microcracks     |
| fracture spacing | 0.4m            | /               | 0.4m            | 4.0m            | 0.1m            |

The initial and boundary conditions are set below: vertical and horizontal in-situ stresses follow the relation $\sigma_v = 30 + 25.5z$, $\sigma_h = 1.3 + 24.9z$, the units of $z$ and stress are m and kPa; depth-dependent initial pore pressure and temperature distributions are shown in Figure 1; nil normal displacements are on the lateral and bottom boundaries. Water is continuously injected into the injection well with a constant rate of 70kg/s at a temperature of 70$^\circ$C, the mass flux of the production well is the same as the injection well.

Figures 2 and 3 show the evolution of production temperature and pressure difference between injection well and production well under different cases (as listed in Table 2). Figure 4 depicts the variation in horizontal permeability of surrounding rocks in injection well during 40-year of heat extraction. Note that the results mentioned are obtained from the center of each well. After 40 years, the horizontal permeability contributed by microcracks along the horizontal line between the center points of two wells is shown in Figure 5.
the maximum value of 127.67°C when only microcracks are considered, while gets the minimum value of 123.12°C in multi-scale structures considered case with dense spacing of fractures.

Figure 4 illustrates that the permeability of fractured rocks during heat extraction increases obviously in the early stage, which results from the decrease of normal effective stress due to the effects of injected water pressure increase and temperature reduction-induced material shrinkage. Affected by the geometries of void structures, the increment of horizontal permeability is larger in the fractures considered case than the solely microcracks considered case, and the effect is amplified by the density of fractures. The more concentrated the fractures are, the less contribution the microcracks make to the permeability of fractured rocks, as shown in Figure 5.

5. Conclusions
In this paper, a damage constitutive and associated permeability evolution model under T-H-M coupled loading is formulated for saturated fractured rocks containing microcracks in rock blocks separated by fractures in the thermodynamic framework. It can consider the effect of multi-scale structures (microcracks and fractures) variation on mechanical and flow behaviors. The coupled T-H-M modeling approach is implemented via linking the proposed model with the fluid flow and heat transfer modeling code, TOUGHREACT, and the effect of the multi-scale structures on the T-H-M coupling responses is examined by simulating the heat extraction of a deeply-buried geothermal project.

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