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Chemically- and Mechanically-mediated Influences on the Transport and Mechanical Characteristics of Rock Fractures

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Abstract

A model is presented to represent changes in the mechanical and transport characteristics of fractured rock that result from coupled mechanical and chemical effects. The specific influence is the elevation of dissolution rates on contacting asperities, which results in a stress- and temperature-dependent permanent closure. A model representing this pressure-dissolution-like behavior is adapted to define the threshold and resulting response in terms of fundamental thermodynamic properties of a contacting fracture. These relations are incorporated in a stress-stiffening model of fracture closure to define the stress- and temperature-dependency of aperture loss and behavior during stress and temperature cycling. These models compare well with laboratory and field experiments, representing both decoupled isobaric and isothermal responses. The model was applied to explore the impact of these responses on heated structures in rock. The result showed a reduction in ultimate induced stresses over the case where chemical effects were not incorporated, with permanent reduction in final stresses after cooling to ambient conditions. Similarly, permeabilities may be lower than they were in the case where chemical effects were not considered, with a net reduction apparent even after cooling to ambient temperature. These heretofore-neglected effects may have a correspondingly significant impact on the performance of heated structures in rock, such as repositories for the containment of radioactive wastes.

Keywords: chemo-mechanical coupling, fracture aperture, fracture constitutive model, rock fracture

1 Introduction

The mechanical and hydraulic properties of rock fractures are of great interest in a wide variety of geological applications, including the long-term disposal of radioactive wastes, the recovery of geothermal energy from engineered geothermal systems (EGS), CO_2 sequestration in saline aquifers and petroleum reservoirs, and the fracturing and faulting of rocks [1]. In particular, in crystalline and volcanic rocks, the fractures have much higher permeability and compliance than the surrounding rock matrix, and therefore the fractures represent dominant conduits for fluid transport and for mechanical deformation. In these applications, the capacity of fractures to transmit fluid plays a significant role in the performance of structures constructed on and in rock.

Importantly, the transmission and mechanical characteristics of natural fractures evolve constantly and can be considered as dynamic variables [1]. Individual thermal, mechanical, hydraulic, and chemical processes elicit particular responses and influence fracture apertures, with these influences resulting both from natural stressors and human activities. Changes in fracture aperture in turn change permeability, with the cubic dependency on aperture resulting in a high degree of sensitivity to small perturbations [2]. An important consideration for the analysis of fluid flow and transport is that fracture permeabilities cannot be treated as a constant parameter, especially when large changes in thermal, mechanical, and chemical conditions are anticipated.

As for mechanical mediation, fractures can close or open as a result of mechanical stresses induced by numerous sources including excavation, changes in effective stress and thermal expansion [1]. Diminution of aperture is caused by compressive normal stresses, and extensional or shear-dilational effects give rise to increases in aperture [3-5]. Previous investigations suggest that changes in permeability, even due to modest changes in stresses, may reach a few orders of magnitude [5, 6]. To date, most studies have focused on mechanically-mediated changes, and these studies have produced a number of constitutive equations to account for the effects of mechanical stress on fracture aperture [3, 7, 8].

Compared to the mechanisms and models for the mechanically-mediated changes, the understanding of chemically-mediated changes in permeability is meager. Chemically-mediated changes are known to be important even at relatively modest stresses, temperatures and typically for systems pushed far from chemical equilibrium, such as in geothermal or hydrocarbon reservoirs or around waste repositories. Sealing has been suggested in some instances of vapor and fluid transport under stressed conditions [9-13], and gaping has been suggested in carbonate rocks , e.g., [14]. The controlling processes and feedbacks apply, in varying degrees, to a variety of disciplines, and at a variety of spatial and temporal scales. The changes result mainly from dissolution and precipitation of minerals within the fracture [12-14], both in free-face dissolution and by stress-mediated effects.

Mechanisms of pressure solution may offer an explanation for such a change in permeability under net dissolution with this effect exacerbated under increased temperatures. Pressure solution occurs under the action of non-zero effective stress, and the driving force for inter-granular pressure solution is the stress-induced gradients in chemical potential, which results in solubility gradients in the solid around individual grains. Pressure solution involves the serial processes of dissolution at highly-stressed, mineral contacts, the diffusive transport of dissolved mass along the contact boundaries, and, ultimately, the precipitation of mineral mass on available free faces [15-19]. While pressure solution is an efficient compaction mechanism leading to porosity and permeability reduction in porous rock and aggregates, the significant role of pressure solution has also been observed on fracture permeabilities [12-13].

For example, isobaric laboratory tests on Novaculite [12] have shown a decrease in aperture with temperature increases up to 150 °C despite net dissolution. Similar observations have been reported for in situ tests on gneiss [20] where aperture magnitude was reduced by more than three times as the temperature increased from 12 °C to about 74 °C, again under *invariant* stresses. This behavior cannot be explained by conventional, mechanically-mediated models, and the additional deformation, also termed *over-closure* [21], requires a feasible explanation.

Further, chemically-mediated change is expected to have impact on the distribution of stress during the full cycle of loading-unloading or heating-cooling due to the additional removal of material by dissolution and is impacted by its irreversibility. This change in aperture and stress after unloading or cooling can have important implications for many applications, including nuclear waste repositories where an understanding of the behavior during thermal cycling is of direct interest for performance assessment. Recently, some models have been developed in studies of the chemo-mechanical effects on transport properties, and these models have been applied to quantify the rates of fracture closure at a given stress condition [12-14]. The current work focused on different aspects of chemo-mechanical effects on fractured rock by considering the steady-state aperture changes that occur during the loading and unloading history of mechanical stress and temperature. In this study, we also investigated the change of mechanical behavior of fractured rock triggered by the permanent reduction of fracture aperture. This improvement enabled us to implement this model for a large-scale analysis, such as the performance assessment of a geological repository of nuclear waste.

The goal of this paper is to provide a combined and integrated model for the evolution of fracture apertures for both mechanically- and chemically-mediated changes to investigate the possible change of permeability and associated stress evolution during the full cycle of heating and cooling and related loading and unloading. In the following, we develop a consistent model to explain the evolution of such stress and chemically-mediated changes of aperture in addition to mechanically-mediated changes. These models are based on stress-elevated chemical potential, and, from a mechanistic basis, they are able to explain thermal and stress dependencies of observed responses. The developed model is then applied to available laboratory and in-situ experiments with isobaric temperature change and isothermal stress change for validation. The proposed model is implemented in a confined, one-dimensional model with fractures subject to a thermal loading-unloading cycle to show the possible range of stress and aperture change.

2 Chemically- and Mechanically- mediated Changes in Aperture

A model was developed to represent changes in fracture aperture mediated by chemical and mechanical processes. The interaction between the various processes that contribute to the response of fracture aperture is illustrated in Fig. 1. Direct changes in total stress, as well as thermally- and hydraulically-induced changes in effective stresses, may develop changes in aperture by mechanical closure or opening. Chemically-mediated changes can be induced by pressure solution-type behavior due to changes in stress or temperature that affect both dissolution and precipitation and that have concomitant influences on fracture aperture. The crucial distinction in this is to note that direct mechanical effects and indirect effects mediated by dissolution must be considered separately. This study only models the pressure solution occurring at the edge of fracture asperity and is concerned only with the case in which fracture permeability decreases. It is also recognized that there can be an increase of permeability by free face dissolution, but this process is not applicable for the proposed model. [14].

In the following, we develop representative expressions to combine each of these effects into a coherent response.

2.1 Mechanical Effects

Various constitutive relationships in linear, hyperbolic, or logarithmic forms are available to represent fracture closure under applied stress, e.g., [3, 7, 8]. The nonlinear form is advantageous in that it can represent the observed stiffening of fractures with closure. One simple, nonlinear relationship that accommodates this observed stiffening is the exponential form shown below [23]:

$$b_m = b_{mr} + (b_{mo} - b_{mr})\exp(-\alpha\sigma) \tag{1}$$

where b_m represents the aperture resulting from mechanical effects alone; b_{mo} is the aperture under a small reference stress; b_{mr} is the residual aperture; and α is a constant related to the nonlinear stiffness of the fracture. The applied stress is σ, and the difference between b_{mo} and b_{mr} is the maximum deformation, $b_{\max}$ [23].

2.2 Chemical Effects

Superimposed on the effect of applied stresses is the influence of chemically-mediated changes in the aperture. This transforms the mechanical aperture b_m where the influences of thermo-chemical and mechano-chemical processes may be combined at the contact areas between the surfaces of the fracture [13]. This enables the aperture to be defined as:

$$b = b_r + \left(b_m - b_r\right)\exp\left[-(R_c - R_{c0})/a\right] \tag{2}$$

where b_r is residual aperture; R_c is the contact area ratio; R_{co} is the reference contact area ratio; and *a* is a constant. The contact area ratio is the ratio of the contacting or inter-penetrating fracture as a proportion of the total fracture area. This relation notes the exponential relation between fracture closure and contact area, which was apparent in observations [13].

From force equilibrium, the contact area ratio can be defined as:

$$R_c = \frac{A_a}{A} = \frac{\sigma}{\sigma_a} \tag{3}$$

where A_a is the total contact area; A is the total area subject to the macroscopic stress; σ is the macroscopic effective normal stress applied on the fracture; and σ_a is the microscopic normal stress realized on the asperity contacts. Dissolution of the contacting asperity will progress when the local asperity stress exceeds a critical stress.

The value of critical stress was estimated as a fraction of heat fusion at a grain-to-grain contact without considering the temperature dependence [24]. Considering the temperature change, the critical stress, σ_c, is defined as [25-26]:

$$\sigma_c = \frac{E_m \left(1 - T / T_m\right)}{4V_m} \tag{4}$$

where E_m is the heat of fusion; T is temperature; T_m is the temperature of fusion; and V_m is the molar volume of the mineral comprising the fracture asperity. This critical stress defines the stress state where the compaction will effectively stop [25], and it can be viewed as a threshold stress. In other words, dissolution of asperity contacts will continue as long as the microscopic stress exceeds the critical stress. The aspect of the dependency of this critical stress on temperature was discussed elsewhere [27].

The equilibrium contact area at the completion of the compaction process in steady state is defined as:

$$R_f = \frac{A_f}{A} = \frac{\sigma}{\sigma_c} \tag{5}$$

where R_f is the final contact area ratio when pressure solution halts, and A_f is the final contact area.

The increase of contact area ratio and the resulting change in the aperture are illustrated schematically in Fig. 2, and the reduction of aperture will continue until the contact stress is equal to the critical stress due to the increase of contact area. The final contact area ratio R_f is the summation of all final contact area ratios defined as follows:

$$R_f = \frac{1}{A}\sum_{i=1}^{n} A_{fi} \tag{6}$$

where n is the number of discrete contact points.

Because we are considering the final reduction of aperture at steady state, Eq. (5) is equated with the contact area ratio (R_c). Inserting Eq. (5) into Eq. (2) yields:

$$b = b_r + (b_m - b_r)\exp\left\{-\left(\frac{\sigma}{\sigma_c} - R_i\sigma\right)/\,a\right\} \tag{7}$$

In the above equation, the reference contact area ratio (R_{co}) is redefined as a stress dependent form using the index contact area ratio (R_i) as a proportionality constant in order to consider the fact that the reference contact area ratio is actually dependent on the macroscopic stress.

Inserting Eq. (1) into Eq. (7) yields:

$$b = b_r + \left\{ b_{mr} - b_r + (b_{mo} - b_{mr}) \exp(-\alpha\sigma) \right\} \exp\left\{ -\left(\frac{\sigma}{\left(\frac{E_m \left(1 - T/T_m\right)}{4V_m} \right)} - R_i\sigma \right) / a \right\} \quad (8)$$

In the interest of simplicity, the term used to represent the pressure solution type behavior may be simplified as:

$$\left(\frac{\sigma}{\left(\frac{E_m \left(1 - T/T_m\right)}{4V_m} \right)} - R_i\sigma \right) / a = \left(\frac{4V_m T_m / E_m}{\left(T_m - T\right) a} - R_i / a \right) \sigma \approx \left(\beta - \frac{\gamma}{T} \right) \sigma \qquad (9)$$

These coefficients may be inserted into Eq. (8) leading to a simpler form:

$$b = b_r + \left\{ b_{mr} - b_r + (b_{mo} - b_{mr}) \exp(-\alpha\sigma) \right\} \exp\left\{ -\left(\beta - \frac{\gamma}{T} \right) \sigma \right\} \qquad (10)$$

This relationship embodies the important influence of mechanical effects alone, included in the first exponential term, and those mediated by stress- and thermally-activated changes in the chemical response. The equation can be presented in a form where independent parameters are readily recognizable:

$$b = b_r + \left\{ b_{mc} + b_{\max} \exp(-\alpha\sigma) \right\} \exp\left\{ -\left(\beta - \frac{\gamma}{T} \right) \sigma \right\} \qquad (11)$$

where $b_{\max}$ is the maximum mechanical deformation of the aperture, and b_{mc} is the difference between the residual mechanical and residual chemical apertures. The complete constitutive response is presented schematically in Fig. 3.

Notably, the relation in Eq. (11) represents the equilibrium behavior where the closure process has evolved to an equilibrium state at a given increment of temperature and stress.

When there is no difference between mechanical and chemical residual aperture, i.e., $b_{mr} = b_r$, the equation reduces to:

$$b = b_r + b_{\max} \exp(-\alpha\sigma) \exp\left\{ -\left(\beta - \frac{\gamma}{T} \right) \sigma \right\} \qquad (12)$$

With the knowledge of fracture geometry, this suggested equation can be incorporated into the deformation and hydraulic analyses at a larger scale to investigate the effect of fracture aperture change in fractured rocks. Because the exponential form of aperture change results in nonlinear constitutive relation, hydraulic or mechanical analyses at a larger scale should be conducted in a fully nonlinear fashion.

2.3 Fracture Unloading

In addition to fracture loading, reductions in stresses or temperature also elicit responses in the aperture. An important consideration is that, during unloading, the fracture does not recover fully, due to irrecoverable plastic deformation [28] and removal of material by dissolution from beneath contacting asperities. In order to include the partial reversibility of the mechanically- and chemically-mediated changes in the aperture, a recovery ratio is defined as the ratio of maximum recovery of aperture due to unloading and cooling ($b^u{}_{\max}$) relative to the maximum closure ($b_{\max}$):

$$R = \frac{b^u{}_{\max}}{b_{\max}} \tag{13}$$

When a fracture is unloaded at a certain stress, the change in the aperture of the unloaded fracture is a function of both stress and temperature:

$$b^u(\sigma, T) = (1 - R) \cdot b(\sigma^u, T^u) + R \cdot b(\sigma, T) \tag{14}$$

where σ^u and T^u are the stress and temperature, respectively, at the initial unloading and cooling, i.e., at the turning point from loading to unloading or from heating to cooling. The form of this expression is represented schematically in Fig. 4.

This shows that the degree of recovery is a function of the stress at which the fracture is unloaded, i.e., the higher the initial unloading stress, the smaller the unloaded aperture. Similarly, the aperture is a function of the initial cooling temperature.

For a recovery ratio of unity, the deformation is fully recoverable upon unloading, and it follows the original loading path, but in reverse. When the recovery ratio is zero, the fracture retains the same aperture as that reached at maximum closure, and it remains invariant with reductions in either stress or temperature.

Combining these loading and unloading effects, the full description of unloading and cooling behavior may be represented by inserting Eq. (12) into Eq. (14):

$$b = b_r + (1 - R) b_{\max} \exp(-\alpha\sigma^u) \exp\left\{-\left(\beta - \frac{\gamma}{T^u}\right)\sigma^u\right\} + R b_{\max} \exp(-\alpha\sigma) \exp\left\{-\left(\beta - \frac{\gamma}{T}\right)\sigma\right\} \tag{15}$$

where the sequential terms represent the loading and unloading portions, respectively.

Incorporation into deformation and hydraulic analyses of a larger scale is also possible to investigate the effect of irreversibility of fracture on deformation and permeability evolution.

3 Application to available data

This prior model, representing the anticipated influence of dissolution mediated by chemical and mechanical effects, is compared with observations from the few controlled laboratory and in situ experiments that reflect this response. The available data are meager, since deconvolution of the response to mechanical and chemical influences is only possible if temperature and stress are independently controlled and applied.

3.1 Arkansas Novaculite

Prior experimental data are available for flow-through tests on a natural fracture in novaculite [12]. Direct observation of pressure solution was evaluated by favorable comparison of change in fracture aperture with anticipated mass removal rate measured in the experiment. This behavior is also consistent with observations of the sectioned fracture, post-test, where SEM micrographs show dissolution sites and the blunting and welding of asperity contacts in a natural fracture that had been separated prior to the test [22]. Careful characterization of the fracture topography and observations of equilibrium changes in the hydraulic apertures were available for the experiments [12] and were fit to the model of Eq. (15), as itemized in Table 1. While the first three parameters (*α, β, γ*) define the sensitivity to temperature and stress, residual and initial apertures were defined to constrain the overall range of the change of aperture. Since unloading measurements were not available, recovery ratio and stress for initial unloading were arbitrarily chosen to explore the possible ranges of responses. Fig. 5 shows the calculated aperture-temperature relation under various stress conditions and the aperture-stress relation at various temperatures with measured values extracted from the data [12]. For simplicity, no distinction was made between mechanical and hydraulic apertures. At a stress of 2.73 MPa, reasonable agreement was reached between measured and modeled apertures (Fig. 5 (a)). Fracture closure increases both with elevated stress at constant temperature and with elevated temperature under constant stress. As shown in Fig. 5 (b), the reduction is more rapid when stress is increased under higher constant temperature due to the lowering of the critical stress, which, in turn, triggers pressure solution. Fig. 6 shows the various possible responses using the suggested empirical relationship when novaculite is unloaded and cooled. The graph shows that the response to unloading is a function of both recovery ratio and the initial unloading stress.

3.2 Terra Tek Block Test

A second validation example is for a block loading test conducted at the Idaho Springs experimental mine in Colorado, USA [20]. The rock is strong, pervasively jointed, granitic gneiss. The experiment isolated four sides of an experimental block with differential loads applied to the individual faces by flat-jacks and heated by line heaters. The back-calculated change in the aperture, recorded during the experiment at different stresses and temperatures, show reductions in the aperture due to temperature increases at an isobaric condition. This mechanism was explained by improved mating of opposing fracture walls [20]. Re-evaluation conducted recently attributed this to the facts that the temperature at which the fractures were formed was higher than the ambient temperature and that rough joints are over-closed compared with smooth joints [21]. It is our argument here that this over-closure is due partly to pressure–solution-type behavior. No fundamental parameters are available to develop the appropriate constant for the model from first principles, however constants used to fit the data are identified in Table 1.

The extent to which the data fit Eq. (15) is shown in Fig. 7, using the constants of Table 1. The good fit between experimental and model data is apparent. The isothermal loading and the isobaric heating and cooling stages are represented reasonably well. The final isothermal unloading stage is less well represented, and the observation is that the unloading is only partially reversible. The observed recovery of the aperture during the final isothermal unloading stage (i.e., from number 5 to 6) is difficult to reconcile, since the unloading deformation is even greater than the loading deformation - intuitively, an unexpected result. The prescribed model cannot match this particular unanticipated response.

The aperture-temperature relationship under various constant stresses and the aperture-stress relationship under various constant temperatures are shown in Fig. 8. Values extrapolated beyond the limits of the experimental data of 7 MPa and 74 degrees are also shown.

3.3 Ancillary Data

Additional anecdotal evidence of the effect of temperature on the reduction of permeability can be observed in other field and laboratory data. These include the response of a heated-block experiment on fractured, welded tuff in the G-tunnel at the Nevada test site [29] and in laboratory experiments on Carnmenellis granite [8].

In the heated-block experiment (with a block size of 2 m x 2 m x 2 m), the block-center temperature at the mid-plane depth of 1 m was cycled to 48, 69, and then 94 °C in a series of three increments. The test duration was of the order of a year, and fracture aperture was calculated from flow-rate measurements in a packed-off section of a borehole piercing a single fracture. With an increase in temperature to about 100 ^{o}C, the results indicate that the fracture aperture decreased from about 65 μm to 30 μm. At the completion of three thermal cycles, the initial aperture was only 50 μm, which indicated irreversible reduction of the aperture due to cooling. This observation was attributed to possible thermal and chemical actions in which silica may have been precipitated within the fracture [29].

Laboratory experiments with Carnmenellis granite also show changes in fracture aperture response during non-isothermal loading [8]. Loading at elevated temperatures resulted in increased closure. This increased closure may be interpreted in a similar manner to the previous observations for thermally-mediated changes in fracture aperture and, hence, permeability.

Nonetheless, available data are sparse and more experimental evidence under controlled thermal, mechanical, and chemical conditions will be required to corroborate the viability of the proposed model.

4 Anticipated Stress Path During a Cycle of Thermal Loading

In addition to the influence on transport properties, the chemo-mechanically-induced aperture changes may also modify deformation and stress fields. The influence can be significant due to the irreversible deformation associated with the processes, and this is investigated further in the current section. This anticipated effect was explored in a one-dimensional geometry with fractures using both linear and nonlinear exponential model.

4.1 Linear Model

The behavior of the fractured system may be represented by an equivalent medium using equivalent thermo-mechanical and chemo-mechanical parameters. Boundary conditions and geometry are shown in Fig. 9. In representing the mechanical response of the system, total strain is defined as:

$$\varepsilon = \varepsilon_E + \varepsilon_T + \varepsilon_m^j + \varepsilon_c^j \tag{16}$$

where ε_E is the elastic strain of intact rock; ε_T is the thermal strain of intact rock; ε_m^j is the mechanical strain of due to fractures; and ε_c^j is the chemical strain due to fractures.

Each strain is defined as:

$$\varepsilon_E = \frac{1}{E}\sigma \tag{17}$$

$$\varepsilon_T = -\alpha_T (T - T_0) \tag{18}$$

$$\varepsilon_m^j = \frac{\Delta b_m}{S} = \frac{\sigma}{Sk} \tag{19}$$

$$\varepsilon_c^j = \frac{\Delta b_c}{S} = \alpha_c \left(T - T_0\right) \tag{20}$$

where E is the elastic modulus of the intact rock; α_T is the coefficient of thermal expansion of the rock; T_o is the initial temperature; Δb_m is the mechanically-mediated aperture change; Δb_c is the chemically-mediated aperture change; S is the spacing between parallel fractures; and k is the normal stiffness of the fracture. A new parameter that was adopted to account for the pressure-solution type behavior in this study is the linear chemical expansion coefficient, α_c, which relates the change in temperature to the shrinkage in the linear dimension of the material. This linear chemical expansion coefficient is assumed to be a function of only temperature in this particular, one-dimensional problem in order to simplify the case.

The magnitude of an aperture resulting from both mechanically- and chemically-mediated changes is defined as:

$$b = b_0 - \Delta b = b_0 - \Delta b_m - \Delta b_c \tag{21}$$

where b_0 is the initial aperture at zero stress and closure is noted to be positive.

The constitutive equation relating elastic stress to strain is defined as:

$$\sigma = E(\varepsilon - \varepsilon_T - \varepsilon_m^j - \varepsilon_c^j) \tag{22}$$

For a one-dimensional system with a fixed displacement boundary, the problem reduces to:

$$\sigma = E\left\{\alpha_T(T - T_0) - \frac{1}{S}(b_0 - b)\right\} \tag{23}$$

$$b = b_0 - \frac{\sigma}{k} - S\alpha_c(T - T_0) \tag{24}$$

By solving Eqs. (23) and (24) for σ, the result is:

$$\sigma = \frac{ESk}{Sk + E}(\alpha_T - \alpha_c)(T - T_0) \tag{25}$$

From this relationship the induced stress resulting from a change in temperature may be calculated readily.

Fig. 10 shows the paths of temperature-stress and stress-aperture during heating and cooling from a reference case. In this example, the initial stress of 5 MPa rises to 12 MPa with a temperature increase of 100 °C. It is assumed that T is uniform throughout the domain of interest. The maximum stress of 12 MPa is smaller than both the case in which only mechanical effect was incorporated (14 MPa) and the case in which there were no fractures (17 MPa). This is because the reduction of the fracture aperture partially offsets the expansion of the rock matrix. Naturally, when the additional reduction of the fracture due to pressure-solution-type behavior is considered, the generated thermal stress is the lowest of the three cases.

After complete cooling of the system, the stress decreases below the initial stress, since a portion of strain has been irreversibly removed. Because the aperture cannot recover to the initial value, relaxation is necessary in the intact rock, and this causes a greater reduction of the thermal stress upon cooling. When the mechanical change is reversible and the chemically-mediated change is completely irreversible, the final stress reaches about 3 MPa after cooling, which is a reduction of about 2 MPa from the initial stress of 5 MPa. In the extreme case when both mechanical and chemical strains are completely irreversible, the stress can almost become zero at the termination of the heating and cooling cycle. A realistic response would lie between these two cases, noted as numbers 5 and 6 in Fig. 10 (a). The implication of this reduction of final stress after cooling is that there can be a local failure of the discrete block system due to the loss of confinement.

During the heating and after cooling, the permeability of fractured rock, which may be calculated from the aperture with a given fracture geometry, may be reduced over the case in which chemical effects are not considered. An important observation in this study is that the reduction of permanent stress after cooling does not actually result in the increase of aperture. This counter-intuitive phenomenon is explained by the fact that the reduction of the aperture is the actual cause of the stress relaxation in the constrained model. Therefore, the final aperture after cooling cannot be larger than the initial aperture, even with reduced stress.

Finally, this reference case is chosen where the compressive initial stress is present to emphasize the significance of the reduction of stress after cooling. In a system with no initial stress, the final stress would likely become zero because of the tension cut-off in the fracture.

4.2 Nonlinear Model

A similar response can be modeled using the prior nonlinear constitutive equation. As fracture deformation (ε^j) is lumped together in the suggested form, the stress-strain relationship becomes:

$$\sigma = E(\varepsilon - \varepsilon_T - \varepsilon^j) \tag{26}$$

where $\varepsilon^j = \varepsilon_m^j + \varepsilon_c^j$, and $\varepsilon^j = \frac{1}{S}(b_0 - b)$ in one dimension.

From Eqs. (23) and (11), the problem reduces to solving the following two coupled, nonlinear algebraic equations with two unknowns, σ and b:

$$f_1 = \sigma - E\alpha_T(T - T_0) + \frac{E}{S}(b_0 - b) = 0 \tag{27}$$

$$f_2 = b - b_r - \{b_{mc} + b_{\max}\exp(-\alpha\sigma)\}\exp\left\{-\left(\beta - \frac{\gamma}{T}\right)\sigma\right\} = 0 \tag{28}$$

During the cooling stage, the second nonlinear equation has a slightly different form to account for the irreversible responses, i.e.,:

$$
\begin{aligned}
f_2' = b-(1-R)\left[b_r+\left\{b_{mc}+b_{\max}\exp(-\alpha\sigma^u)\right\}\exp\left\{-\left(\beta-\frac{\gamma}{T^u}\right)\sigma_i^u\right\}\right] \\
-R\left[b_r+\left\{b_{mc}+b_{\max}\exp(-\alpha\sigma)\right\}\exp\left\{-\left(\beta-\frac{\gamma}{T}\right)\sigma\right\}\right]
\end{aligned}
\qquad (29)
$$

The solutions of these coupled equations are found by applying Newton's method in a system of nonlinear equations by applying successively a Jacobian of two algebraic equations until the solutions converge [30]. Fig. 11 shows the temperature-stress and stress-aperture relationships during heating and cooling of the one-dimensional system. The parameters used for this analysis were also taken from Table 1 for the Terra Tek block test. The response to cooling (or unloading) within the nonlinear model is, in general, similar to the linear model. Unloading paths were investigated with different recovery ratios. Similar to the linear model, the nonlinear model also shows less of an increase in thermal stress during the loading stage and a greater reduction of thermal stress upon cooling compared with the model in which chemically-mediated change was not considered. The aperture, which can be directly related to permeability of fractured rock, was also less than it was in the case in which chemical effects were not considered. This observation may have important implications where multiple cycles of heating and cooling are superimposed.

5 Conclusions

The model in this paper represents changes in the mechanical and transport characteristics of rock masses as a result of both mechanically- and chemically-mediated changes. Fracture closure is used as the vehicle to define changes in these properties, with stiffness and permeability defined relative to fracture apertures and to changes in these apertures. This response is evaluated for fractures that stiffen with closure, represented by an exponential relationship between fracture closure and applied effective stress.

Dissolution at asperity contacts was incorporated in the evaluation of aperture change, with an activation threshold defined through the concept of a local critical stress, defined relative to the material properties of the contacting minerals. This threshold defines when irreversible chemical effects will initiate and when they will be significant. Since the fundamental parameters that control the evolution of the chemical response are difficult to determine at the rock mass scale, these parameters are recast as empirical coefficients that represent the evolving response. Specifically, these parameters enable the decoupling of chemical effects under invariant stress, for incremented temperature, and under invariant temperature for incremental stress. The utility of this approach was compared with the results of laboratory and field experiments and was shown to adequately fit the observed response. The model was able to match the aperture change observed in novaculite in the laboratory as temperature was increased at an isobaric condition. Comparisons with field experimental data show a reasonable agreement in isothermal loading and isobaric temperature changes. Importantly, these matches cannot be achieved with models of mechanically-mediated change alone. Further, this model can be used to determine the evolution of the deformation and hydraulic characteristics at a larger scale to investigate the up-scaled effect in fractured rocks.

These observed behaviors were explored for a mechanically-constrained, one-dimensional model subject to a thermal loading-unloading cycle. The results showed that chemically-mediated change tends to reduce thermal stress during the loading stage and, interestingly, a permanent reduction in stress upon cooling. The thermal stress generated is smaller than where chemical effects are absent, because the reduction in the aperture due to temperature increase partially offsets the expansion of the intact rock. The permanent reduction of stress upon cooling was explained by the irreversible change of the aperture. During the heating and after cooling , the permeability of fractured rock may also be reduced over the case in which chemical effects are not considered. This reduction of permeability even with reduced stress was explained by the fact that the reduction of the aperture is the actual cause of the stress relaxation in the constrained model.

The implication of these behaviors is important since thermal stresses are reduced over anticipated magnitudes, and a permanent reduction in stress may result in the loss of keying around underground excavations where local failure may be more likely due to the loss of confinement. Furthermore, the observed evolution of permeability may have a significant impact on the performance of heated structures in rock, such as repositories for the containment of radioactive wastes.

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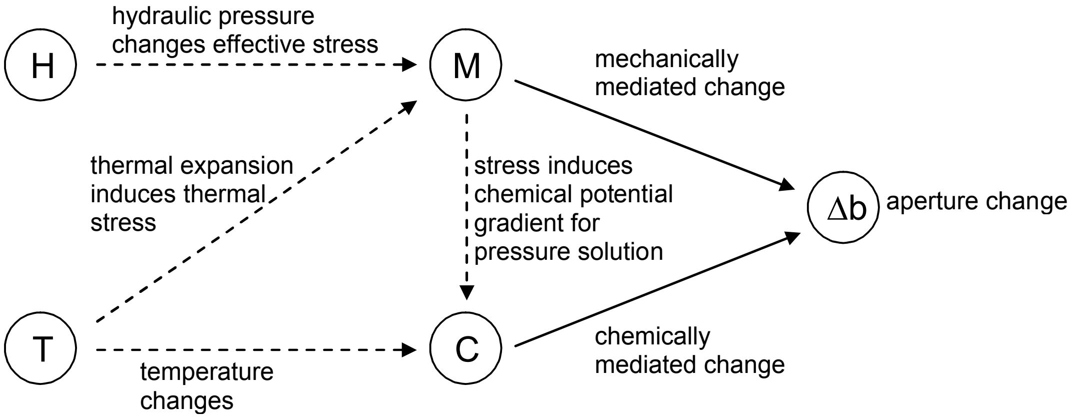


Fig. 1. Thermo-mechanical-chemical interactions described in schematic form to represent chemically- and mechanically- mediated changes in aperture that then contribute to changes in transport or mechanical properties. Mechanically mediated change includes deformation due to mechanical stress and chemically mediated change includes dissolution and precipitation.

Figure2

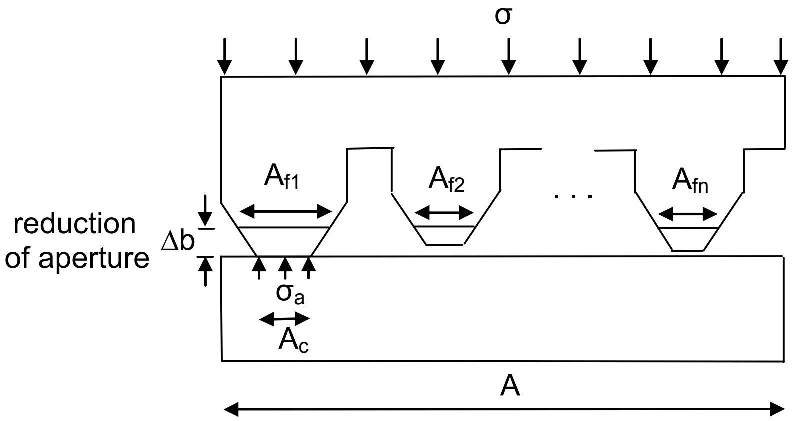


Fig. 2. A conceptual model of aperture geometry for the contact area ratio-aperture relationship with the number of discrete contact points n. Aperture decreases until the contact area becomes large enough for the contact stress (σ_a) to be equated with the critical stress.

Figure3

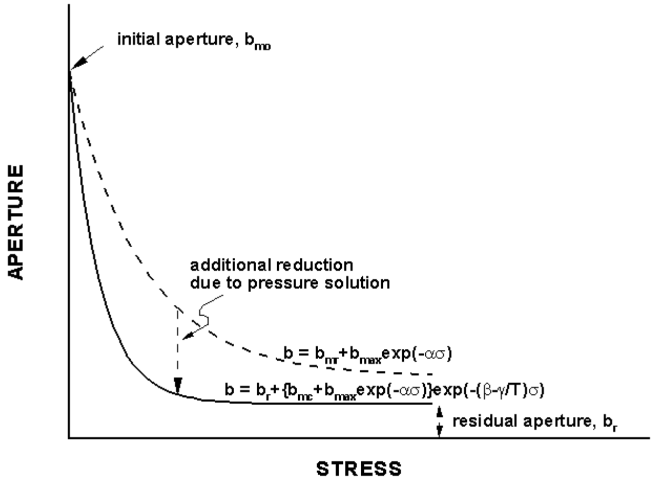
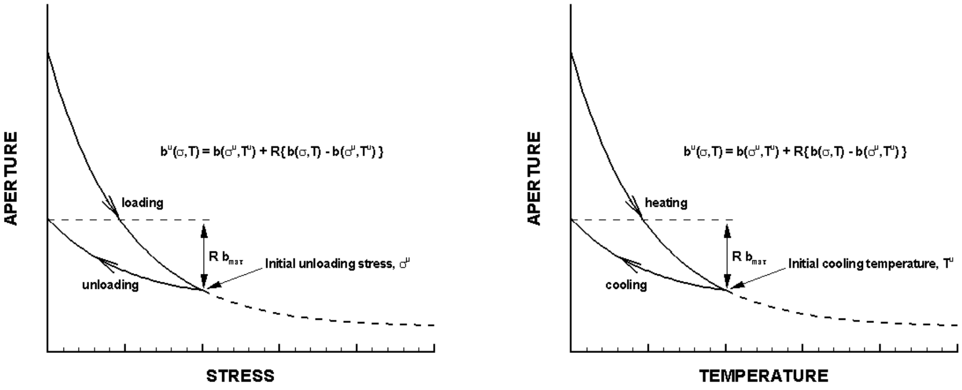


Fig. 3. Fracture aperture model under applied stress with both chemically- and mechanically- mediated change

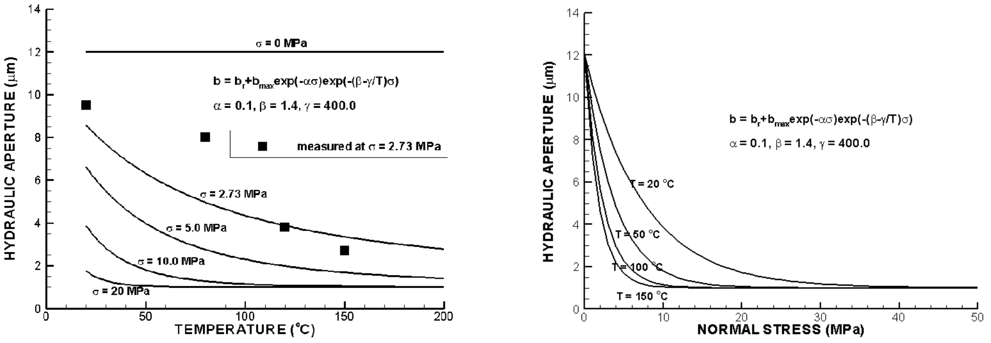
Figure4



(a) (b)

Fig. 4. Fracture aperture model of unloading and cooling

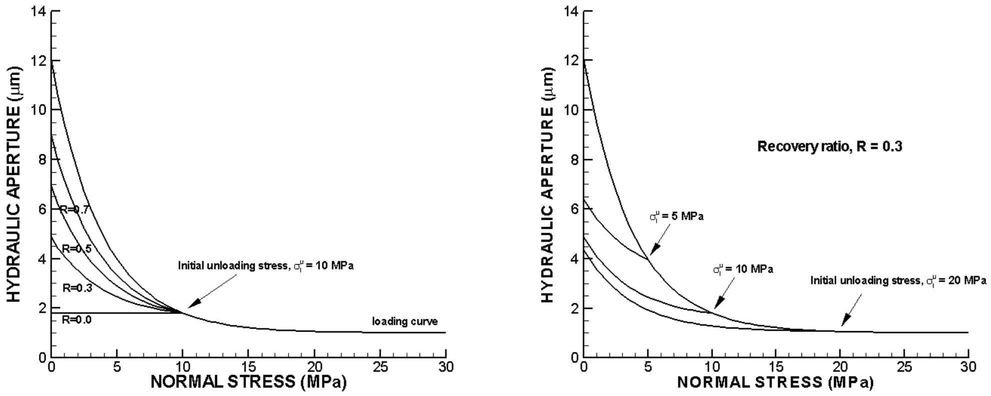
Figure5



(a) (b)

Fig. 5. Change of aperture with respect to temperature and normal stress calculated by the suggested model. Measured aperture is compared in Fig. 5(a)

Figure6



(a) (b)

Fig. 6. Unloading path of both mechanically- and chemically-mediated change of aperture with (a) different recovery ratio and (b) initial unloading stress

Figure7

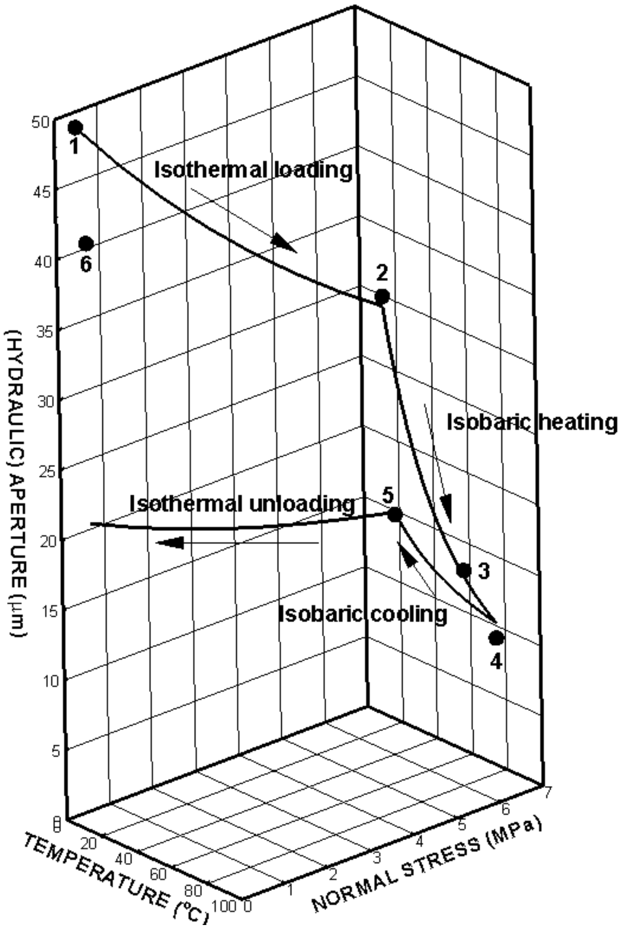
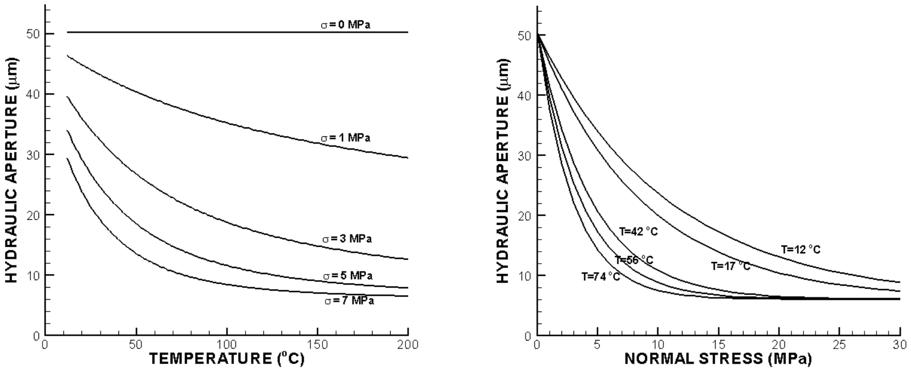


Fig.7. Aperture changes with stress and temperature. Terra Tek measurements are denoted by filled circle and each number follows the sequential stages of changes of stress and temperature. Good agreement is achieved except for the last measurement point (number 6), which seems to be unreasonably high.

Figure8



(a) (b)

Fig. 8. Projected change of apertures from Terra Tek block test (a) isobaric temperature-aperture relations and (b) isothermal stress-aperture relations

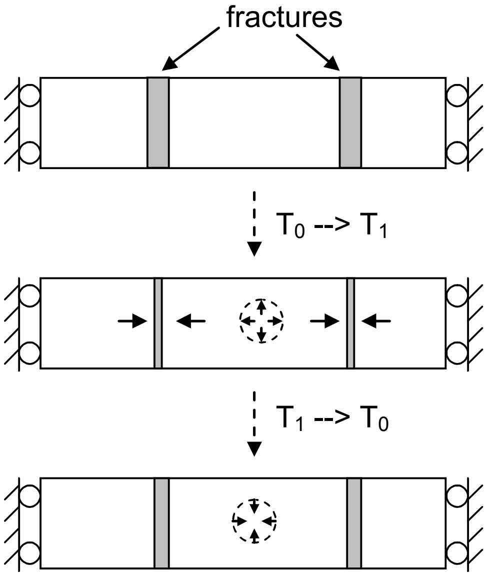
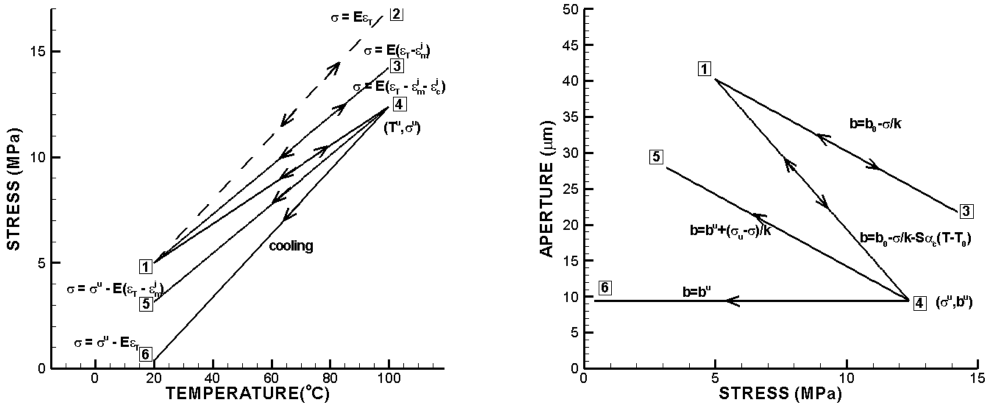


Fig. 9. One-dimensional fractured model with fixed displacement boundary under heating and cooling. It is assumed that a large number of fractures exist in the model at equal spacing. Initial temperature (T_0) was increased to a higher temperature (T_1) and then reduced. After cooling, the closed fractures do not recover to the initial aperture.

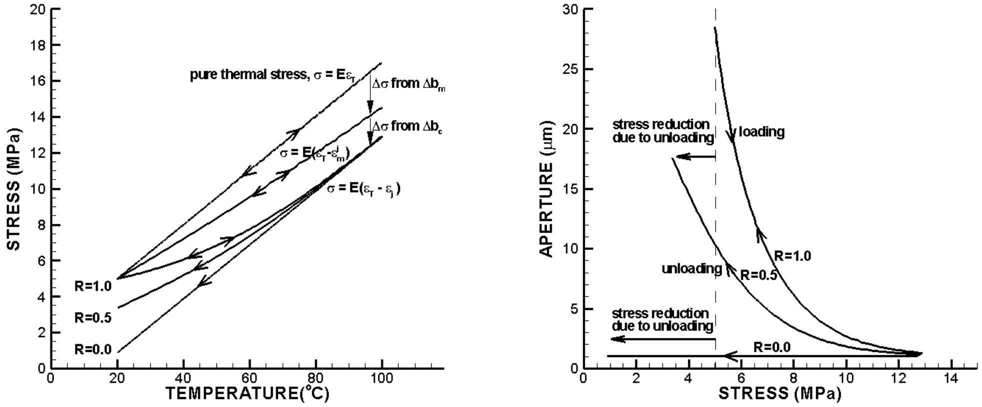
Figure10



(a) (b)

Fig. 10. Paths for temperature-stress and stress-aperture relation for linear stiffness and chemical dissolution model. The listed numbers connect various paths with 1 to 2 noting response on intact rock and the other paths with fractures. For the thermomechanical loading path, 1 to 3 path designates response with only mechanical effect in the fracture, 1 to 4 with both mechanical and chemical effect. For unloading paths, 4 to 1 designates responses with full recovery, 4 to 5 with recovery in intact rock and mechanical effect in fracture, and 4 to 6 with recovery only in intact rock. The parameters used in this Figure are: elastic modulus, E = 15 MPa; spacing, S = 0.1 m; normal stiffness of a fracture, k = 500 GPa/m; thermal expansion coefficient, α_T = 0.1 x 10^{-6} /°C; chemical expansion coefficient, α_c = 2 x 10^{-6} /°C; initial temperature, T_o = 20 °C; initial stress = 5 MPa; and initial aperture at zero stress, b_0 = 50.2 μm.

Figure11



(a)

(b)

Fig. 11. Paths of temperature-stress and stress-aperture responses during heating and cooling stages

Table 1. Parameters that were obtained from flow-through test on Arkansas novaculite and Terra Tek block test.

Parameters	Arkansas novaculite	Terra Tek block test
Constant defining mechanical behavior, α (1/MPa)	0.1	0.1
Constant defining chemical solution, β	1.4	1.36
Constant defining chemical solution, γ	400	390
Residual aperture under mechanical stress alone, b_{mr} (μm)	1	6
Residual aperture under chemical solution, b_r (μm)	1	6
Initial aperture, b_{mo} (μm)	12	50.2
Recovery Ratio, R	0.3	0.3